

SERMACS 2023

WEDNESDAY MORNING

Durham Convention Center
Junior Ballroom B

Shining a Light on Synthetic Fuels

Cosponsored by ENFL
D. Kurtz, A. J. Miller, *Organizers, Presiding*

8:30 Welcome and Introduction of Keynote Speaker.

8:35. Single-molecule panchromatic photocatalysts for hydrogen production with red light. **C. Turro**

9:20 Q&A with Prof. Turro.

9:30 Introductory Remarks for Shining Light Session.

9:35. An electrocatalytic cascade sequence for the reduction of CO₂ to methanol. **S. Fernandez**, E.A. Assaf, S. Ahmad, N. Hazari, M.Z. Ertem, A.J. Miller

9:45. Relevance and reactivity of a ferrous carbonyl intermediate in porphyrin-mediated CO₂ reduction. **K. Luedecke**, R.G. Hadt

9:55. Mediating thermodynamically challenging reactions with earth-abundant chromium(III) photocatalysts. **A.T. Barth**, F.N. Castellano

10:05 Early Career Researcher Discussion.

10:25 Intermission.

10:45. Making methanol from metal carbonyl complexes. **R.N. Sampaio**, A. Muller, J.T. Sirlin, M.Z. Ertem, D.E. Polyansky, D.C. Grills, G.J. Meyer, J.J. Concepcion

11:05 Speaker 4 Q&A.

11:10. From captured CO₂ to value-added chemicals: A photochemical approach. **K. Glusac**

11:30 Speaker 5 Q&A.

11:35. Direct Photochemical C–H activation and C–C bond formation toward the production of energy dense fuels. S. Fosshat, S.M. Siddhiaratchi, C. Baumberger, V.Z. Valley, **M.B. Chambers**

11:55 Speaker 6 Q&A.

Durham Convention Center
Grand Ballroom I

Biochemistry Research and Development Poster Session

Cosponsored by BIOL
D. A. Canelas, K. C. Glasgow, *Organizers*

9:00 - 11:00

101. Development of an alternative medium for the growth of *Lactobacillus delbrueckii* ssp. *bulgaricus* [Poster Board #101]. **P. YEBOAH, S. Ibrahim, N.D. WIJEMANNA, A.A. EDDIN, A. Brock**

102. A study of the biochemistry of *Zingiber Officinale* (Ginger Root): A widely used diabetes remedy [Poster Board #102]. **S. Sosa**, A. Mar, H. Morales, E. Plata

103. Investigating the cell penetration of proteins and lipid nanoparticles (LNPs) with the chloroalkane penetration assay (CAPA) [Poster Board #103]. **J. Wang, J. Kritzer**

104. Synthetic lectins for the determination of breast cancer subtype by flow cytometry [Poster Board #104]. **J. Boyt**

105. Wastewater treatment using microbial fuel cell technology [Poster Board #105]. **D. Bing**, D. North

106. Optogenetic regulation of EphA1 receptor activation and signaling [Poster Board #106]. **A. Wurz**, R. Hughes

107. Using native lipids to formulate reverse micelles for understanding peripheral membrane proteins [Poster Board #107]. **S. Walters**, A.J. Castillo, C.L. Labrecque, A. Develin, Y. Qu, B. Fuglestad

- 108.** Measuring cellular mechanics using image analysis techniques to provide evidence for a molecular pathway involving obscurin [Poster Board #108]. **S. Ouderkirk**, K.D. Shultz, C.J. Miller, N.T. Wright
- 109.** Hydrogen tunneling in biochemistry lab: Introducing undergraduate students to quantum biology research in the classroom [Poster Board #109]. **E. Brinkley**, A.R. Offenbacher, e. anderson, J.P. Walker
- 110.** Biochemical and structural studies of unusual lipoxygenases from pathogenic fungi [Poster Board #110]. **S.G. Hill**, a. sharma, C. Whittington, B.M. Hoffman, A.R. Offenbacher
- 111.** Investigating Phytosulfokine trafficking: Insights into the role of phytohormones in plant signaling [Poster Board #111]. **M. Tindi**
- 112.** Characterization of dGTPase enzyme function in E.coli with the cysteine-273 to serine mutation using molecular dynamics simulations [Poster Board #112]. **A. Granger**, L. Perera, R. Schaaper
- 113.** Elucidating the role of copper in protein stability and aggregation [Poster Board #113]. **T. Outlaw**, A. Robison, I. Williams, S. Repala, D. Diaz, K.J. Franz
- 114.** Design and synthesis of small molecules as potential cancer therapeutics [Poster Board #114]. **A. Seymour**, C. Peterson, J. Kocerha, K.S. Aiken
- 115.** STORM super-resolution imaging of cytoskeleton effect of f-actin with the calcium signaling in mesothelial cells adhesion assay [Poster Board #115]. **J. Chen**
- 116.** Unraveling phytosulfokine trafficking in *Arabidopsis thaliana* using fiber-optic fluorescence microscopy [Poster Board #116]. **I. Obuaba**
- 117.** Prediction of pKa of modified nucleobases using Molgpka [Poster Board #117]. **H. Chowdhury**, N. Chiu, F. Morales Shnaider
- 118.** The effects of net dye charge on DNA photocleavage at 750 nm by donor-acceptor fluorophores [Poster Board #118]. **C. Seudieu**, G.E. Özmen, D. Brewer, M. Henary, K.B. Grant
- 119.** Thermodynamics of 5'-GGGGCCCC-3' binding to Neomycin-class aminoglycosides [Poster Board #119]. **A. Conner**, M. Fuller, P. Kellish, D.P. Arya
- 120.** Kinetics of peroxidase (POD) and polyphenoloxidase (PFO) inactivation in blackberry fruits (*Rubus glaucus*) [Poster Board #120]. **D. Rodr?iguez**, J.E. Granados
- 121.** Targeted ¹H-NMR-based metabolomics analysis of serum markers of fatty liver in the glucose intolerant, hyperinsulinemic male LEW.1WR1 rat model [Poster Board #121]. **E.C. Hunt**, S.T. Love-Rutledge, B.W. Vogler

- 122.** QM-cluster modeling for chorismate mutase based on sampling MD simulation [Poster Board #122]. **D.A. Agbaglo, T. Summers, Q. Cheng, N.J. Deyonker**
- 123.** The production of DNA damaging reactive oxygen species by some natural products: A comparative analysis [Poster Board #123]. **E.A. Obayuwana, K.B. Grant**
- 124.** Spectroscopic studies of mineralized horse heart cytochrome c within a zeolitic imidazole framework [Poster Board #124]. **B. Wolfe, D. Lund, R.W. Larsen**
- 125.** Enhancement of plastic degradation by the bacterium *Ideonella sakaiensis* [Poster Board #125]. **T.D. Gruber, M.K. Lorenger, C.R. Salazar, L. Le, J. Reed**
- 126.** Combating bacterial biofilms: Investigating unconventional regulatory proteins SypA and SypE in *Vibrio fischeri* [Poster Board #126]. **E.M. Bensch, K. Gaddy, E. Abhulimen, M. Milton**
- 127.** Development of multifunctional hemoglobin Dehaloperoxidase (DHP) from *amphitrite ornata* as a versatile biocatalyst for diverse substrates [Poster Board #127]. **D. Yun, R.A. Ghiladi**
- 128.** Probing the assembly of bacterial non-heme ferritin by site-directed mutagenesis [Poster Board #128]. **D.F. McCain, H. Arnold, J. Cox, D. Hamner**
- 129.** Inhibition of mold growth and aflatoxin formation by essential oils in stored organic corn grains [Poster Board #129]. J. Yu, E. Iwayemi, **D. Rehrh, S. Davis, L. Williams**
- 130.** ACE-inhibitory activity of extensively hydrolyzed peanut protein concentrate [Poster Board #130]. **S. Poddar, J. Yu**
- 131.** BURP peptide cyclases are responsible for the biosynthesis of a new class of plant RiPPs [Poster Board #131]. **M. Pasquale, S. Hematian, S. Lima, J.R. Chekan**
- 132.** Engineering of new biosynthetic enzymes for ribosomally synthesized and post-translationally modified peptides (RiPPs) [Poster Board #132]. **A.B. Smith, J.R. Chekan**
- 133.** Synthesis and characterization of silver nanocluster hydrogels [Poster Board #133]. **M. Collins, E. Skelly, K. Afonin**
- 134.** Detecting reactive oxygen species photosensitized by aromatic heterocyclic compounds using bio-physical probes [Poster Board #134]. **v. ogbonna, A. Ugboya, K.B. Grant**
- 135.** Activation of various ERK-KTR/Akt-KTR biosensor constructs in HEK293T cells [Poster Board #135]. **K. Zheng**
- 136.** Optogenetic investigation into the formation of actin-cofilin rods through site directed mutagenesis of the actin ATP-binding pocket [Poster Board #136]. **N. Mann, R.M. Hughes**

- 137.** Application of FRET to detect conformational change in functionally relevant viral RNA targets [Poster Board #137]. **A. Bruce**, A.E. Hargrove
- 138.** Epitranscriptomic variations in different phases of cell growth [Poster Board #138]. **E. Martin**, V. Tang, F. Morales Shnaider, H. Wang, N. Chiu
- 139.** Determining the functional effects of c-Myc heterogeneity in triple negative breast cancer [Poster Board #139]. **Y. Wang**, S. Ting, E. Brunk
- 140.** Overcoming bottlenecks to oxidized terpenes via biosensor-guided engineering [Poster Board #140]. **C. Odhiambo**, G.J. Williams
- 141.** Machine learning of three-dimensional protein structures promotes a functional understanding of genome variation [Poster Board #141]. **K. Shukla**, K. Idanwekhai, S. Ting, E. Brunk
- 142.** Synthetic phycobiliproteins: Light-activated binding of phycocyanobilin by a *de novo* protein [Poster Board #142]. **C. O'Brien**, R. Matthews, L. Spangler
- 143.** Discovery of a novel covalent inhibitor for chikungunya virus nsP2 protease [Poster Board #143]. **E. Merten**, J. Sears, A. Ghoshal, A. Hossain, B. Hardy, N. Moorman, M. Heise, P. Brown, T. Willson, K.H. Pearce
- 144.** Oritavancin and fidaxomicin inhibit the SARS-CoV-2 3-chymotrypsin-like protease (3Clpro) enzymatic activity *in vitro* [Poster Board #144]. **P. Dinh**, **V. Chaudhary**, K. Gowda, G. Dean, J. Wong, D.S. Lewis, V.V. Mody, S. Taval
- 145.** Antibiotics block the proteolytic and deubiquitination activity of SRA-CoV-2 papain-like protease (Plpro) *in vitro* [Poster Board #145]. **G. Dean**, P. Dinh, D.S. Lewis, K. Gowda, V. Chaudhary, J. Wong, V.V. Mody, S. Taval
- 146.** Diphenylpyraline analogs as vascular Ca²⁺ channel modulators [Poster Board #146]. **T. Reeves**, J.J. Harp, V. Pulgar
- 147.** Investigation of androgen receptor binding compounds for targeting prostate cancer cells [Poster Board #147]. **M. Volety**, **M.E. Goldthorpe**, **K.R. Rast**, **A. Varadarajan**, A. Frampton, S. Varadarajan
- 148.** Bioinformatic studies of ThiF-enzymes reveals a novel RiPP natural product in *Streptococcus uberis* [Poster Board #148]. **A. RAJPUT**, K. Butler, J.R. Chekan
- 149.** Bioinformatic guided discovery of new cyclopeptide alkaloids [Poster Board #149]. **D. Kriger**, B. Ampolini, M. Pasquale, J.R. Chekan
- 150.** Self-modification of *Chlamydia* protein associating with death domains (CADD) enhances binding to Fas death receptor [Poster Board #150]. **S.S. Skirboll**, H.N. Phan, T.M. Makris

151. Investigating the mechanism of NSA1 removal from the pre-60s ribosomal subunit by Rix7 through single-molecule FRET [Poster Board #151]. **L.A. Rolband**, I. Slivernail, S. Patil, R. Stanley, S. LeBlanc

152. Determining the genetic factors resulting in Nicotine dependency [Poster Board #152]. **K. Yang**, J. Stanley

Durham Arts Council
Adaron Hall

Analytical Chemistry Research and Development

Cosponsored by ANYL
Z. S. Davis, G. E. Potts, *Organizers*
C. De Alwis, K. Turner, *Presiding*

9:30 Opening Remarks.

9:35. Exploiting microelectrode geometry for comprehensive electrochemical detection of individual exocytosis events at single cells. **C. De Alwis**, D. Denison, L.A. Sombers, G.S. McCarty

9:50. Monitoring dopamine and met-enkephalin fluctuations simultaneously, in real-time, using voltammetry in rat striatum. **J. Berger**, J. Todorov, K. Turner, G.S. McCarty, L.A. Sombers

10:05. Comparing aptamer-modified commercial and in-house electrochemical sensors for on-site cocaine detection. **C. Farling**, J. Perry, Y. Xiao

10:20. Electrochemical detection of fenthion for forensic analysis. **S. Robbins**, C.C. Chusuei

10:35 Intermission.

10:45. Voltammetric measurements of evoked dopamine and hydrogen peroxide fluctuations in rat striatum. **K. Turner**, J. Berger, G.S. McCarty, L.A. Sombers

11:00. Increased cathode capacity of the Ni-Fe battery using sulfide addition. **A. Regmi**, T. Dowell, D. Wipf

11:15. Evaluating the interactions between colorimetric indicators and metal ions in solution. **W. Craig**, A.D. Dukes, E. Campbell

11:30. Investigating the sensitivity of aptamer-based cyanine dye displacement assays. **A. Bacon**, Y. Xiao

11:45. Development of molecular rotational resonance spectroscopy for process development and optimization. **A. Byars**, J.L. Neill, R. Sonstrom, A. Mikhonin

Durham Convention Center
Meeting Room 3

Chemistry Education Research and Practice

Cosponsored by CHED
S. L. Johnson, *Organizer, Presiding*

9:30 Opening remarks.

9:35. Exploring the scientific method in the kitchen: Recipe modification as a means to make chemistry concepts accessible in an undergraduate non-laboratory chemistry course. **J.A. Dabrowski**

9:50. Impact of hands-on outreach activities on the perception of chemistry and knowledge of high school students. **P. Bell**, A. Mallia

10:05. Effect of a summer math intervention on math self-efficacy in general chemistry. **A.G. Roessler**

10:20 Break.

10:30. Supporting chemistry majors in the first-semester transition to college through a first year seminar course: Course design and impact on students. **S.A. Wasileski**, J.M. Schmeltzer

10:45. Reflective practice of undergraduate learning assistants (ULAs) and graduate teaching assistants (GTAs) using the Vitruvian model of reflective practice (VMRP). **M. Roshandel**, E. Cote, C. Randles

11:00. Comparison of cognitive resource usage between organic chemistry I and II students to rationalize compound acidity. **J.G. Liang-Lin**, S. Gao, C.T. Cox

11:15 Break.

11:25. Problem-based learning as a strategy for metacognitive learning of Kinetics of anaerobic biochemical reactions developed in biodigesters. **J.E. Granados**

11:40. Valence: A historical and educational perspective. **E. Rudler**, C. Preston, R.M. Jones

11:55. Implementation of specifications-based grading for Organic Chemistry II at a PUI: What went well, what didn't go so well, and thoughts for the future. **J.M. Karty**

Durham Convention Center
Junior Ballroom D1

Environmental Engineering

Cosponsored by ENVR and I&EC
D. F. Call, L. Pal, *Organizers*

9:30 Introductory Remarks.

9:35. Magnetite nanoparticles dispersed rice husk biochar engineered composite for removal of arsenate and phosphate from water. **H.P. Abeysinghe**, P.M. Rodrigo, T.E. Mlsna

9:50. Comparisons of biochar-supported iron nanoparticles composites synthesized from carbothermal and borohydride reductions. **T.T. Peiris**, J. Pish, T.N. Karunaratne, O. Nayanathara, X. Zhang, S. Gunatilake, T.E. Mlsna

10:05. Innovative upcycling of municipal solid waste (MSW) into high-quality biochar for a sustainable future. **R. Rao**, R. Thiyagarajan, N. Haque, S. Bera, L. Pal

10:20. Novel synthesis of an eco-friendly $\text{MgO} \bullet \text{Al}_2\text{O}_3 \bullet \text{SiO}_2$ - engineered rice husk biochar for Nickel sorption in wastewater. **D.O. Oguntuyi**, P.M. Rodrigo, O. Olabode, A.F. Abdulraheem, C.U. Pittman, T.E. Mlsna

10:35 Intermission.

10:45. Bifunctional zeolite-based composite for removal of "forever chemicals". **J. Del Pilar**, S. Hunyadi Murph

11:00. Transformation and release of nanoparticles (NPS) in surface coatings: A case study in exposure. **J.G. Clar**

11:15. Leveraging hyperspectral imaging for enhanced characterization of municipal solid waste. **M. Salas**, S. Kohakade, R. Rao, L. Pal

11:30. Exploration of household dust by XRF and Raman spectroscopy. **A.F. Callender**, S. Decatur, B. Davis

11:45 Concluding Remarks.

Durham Arts Council
PSI Theatre

Inorganic Chemistry Research and Development

Cosponsored by INOR

D. A. Canelas, K. C. Glasgow, J. M. Harrington, *Organizers*

9:30 Introductory Remarks.

9:35. Investigation of non-collinear spin texture in $\text{MnCoGe}_{1/3}\text{As}_{2/3}$. **I. Campbell**, Y. Wang, J. Clark, X. Wang, M. Shatruk

9:50. Impact of a hemilabile ligand on a catalytic hydroacylation reaction with divergent mechanistic pathways. **J.R. Leguillow**, A. Sargent, A.T. Morehead

10:05. Characterization of a cationic cobalt(II) hydroformylation pre-catalyst and the effect of impurity on its hydroformylation activity. **D.R. Holzkecht**, M.B. Chambers

10:20 Break.

10:30. Synthesis and redox reactivity of novel bimetallic iron complexes supported by bisdipyromethane ligand scaffolds. **N. Giorgi**, K. Searles

10:45. Nitridorhenium (V) PNP complexes as novel frustrated Lewis pair catalysts toward UN-activated olefin hydrogenation. **J.L. Scott**, E.A. Ison

11:00. Sonochemical synthesis of Schiff base coordination complexes. **J. Arami**, T. Jurca

11:15. Probing the biophysical interactions between copper and MUC2. **N.B. Schulte**, N. Reznik, K.N. Chacon, D. Fass, K.J. Franz

11:30 Break.

11:40. Using microwaves to accelerate the preparation of rare earth materials for security inks. **C. Rose**

11:55. NaCl-solid solution strategy toward achieving active electrocatalysts for the oxygen evolution reaction. **p.j. Tukur**, F.J. Tukur, J. Wei, Y. Mo

12:10. Actinide photo-redox chemistry at metal oxide electrodes. **C. Dares**, X. Hou, M. Sheridan, J. McLachlan, J. Gonzalez-Moya, R. LACAU, T.S. Grimes

12:25. Photoinduced inter-cavity energy and electron transfer in a mixed-guest metal organic framework. **R.W. Larsen**, Z.L. Magnuson

Durham Convention Center
Junior Ballroom D3

Molecular Representations to Improve Chemical Modeling and Ontology in Relation to Environmental Chemistry Properties & Outcomes

Cosponsored by CINF

N. Charest, C. Lowe, *Organizers*

A. Williams, *Presiding*

9:30 Session introduction.

9:35. Chemical structures to explorable representations: ChemSTER. **N. Charest**, A. Edelman-Muñoz, C. Lowe, A. Williams

9:50. Chemmaps.com V2 - exploring the environmental chemical universe. **A. Borrel**, A. Unnikrishnan, D. Allen, N. Kleinstreuer

10:05. Interpretable chemical grouping using an automated KNIME workflow. **J. Moreira-Filho**, D. Ranganath, M. Conway, C. Schmitt, N. Kleinstreuer, K. Mansouri

10:20 Break.

10:30. VSSTox: The virtual chemical counterpart to EPA's distributed structure-searchable toxicity database. **C. Lowe**, T. Martin, N. Charest, A. Williams

10:45. Metabolic similarity in read-across prediction: A case study using graph convolutional networks and predicted metabolism information. **B. Hagan**, G. Patlewicz, I. Shah

11:00. Chemical similarity for protein degraders. **D. Fourches**

11:15 Break.

11:25. Salsa: Structurally-aware latent space autoencoder. **A. Tropsha**, K. Kirchoff, T. Maxfield, S. Gomez, K. Popov

11:40. Use of supervised learning approaches with hierarchical fragment-based representations (ToxPrints) to characterize mode-of-action in aquatic fish toxicity. **D.T. Chang**, K.A. Fay, K. Mansouri, K. Markey, J. Prindiville, G. Patlewicz, M. Lewis, M. Shobair, E. Saluck, A. Richard

11:55. Impact of feature selection on QSAR and read-across. **T. Martin**, C. Ramsland, N. Charest, C. Lowe, A.J. Williams

12:10 Session Wrap-up.

Durham Convention Center
Junior Ballroom C

Organic Chemistry Research and Development

Cosponsored by ORGN
D. A. Canelas, *Organizer*
J. Sampson, *Presiding*

9:30 Opening Remarks.

9:35. Data visualization and storage in an academic HTE center. **J. Sampson**

9:50. Deoxygenative strategy for chemical modification of carboxylic acids. **B. Kim**

10:05. Studying non-covalent interactions in organocatalysis by varying electronics on chiral isothiourea catalysts. **C. Harrison, S. Wiskur**

10:20 Break.

10:30. Friedel-Crafts alkylation of indoles and benzofurans with secondary acetates and tertiary alcohols. **H. Xia, B. Bicalho, C.W. Downey**

10:45. N-(4-(2,4-dimethylphenyl)thiazol-2-yl)isonicotinamide via Hantzsch Thiazol condensation. R.E. Lee, **I.G. McDonald, L.D. Shelton**, P.E. Heiple

11:00. Photoconversion of fluorescent 1,2,3-triazoles into indoles. **B. Nusser**

11:15 Break.

11:25. Ferrocene linked xanthene dyes for electrochromic applications. **R.E. Venta**, C.N. Scott

11:40. Dimerizing NIR cyanine fluorophores: Does doubling the fluorophore mean doubling the benefits?. **T.E. Ahmed**, M. Henary

Durham Convention Center
Junior Ballroom A3

PFAS Compound

Cosponsored by ENVR
Financially supported by Nexus
W. Bodnar, A. Brennan, D. Macmillan, K. Renyer, *Presiding*

9:30 Introduction.

9:35. Molecular dynamics simulations of polyfluoroalkyl substance self-assembly behavior on graphene substrates. B. Lamb, M. Gunter, **B. Ma**

9:55. New ideal-gas thermochemical properties for thermal destruction of C₂ to C₈ perfluorinated carboxylic acids. **H. Ram**, T.P. Sadej, C. Murphy, T.J. Mallo, P.R. Westmoreland

10:15. New gas-kinetics mechanisms for thermal destruction of C₂ to C₈ perfluorinated carboxylic acids. **C.C. Murphy**, H. Ram, T.P. Sadej, T.J. Mallo, P.R. Westmoreland

10:35 Break.

10:55. Category-based toxicity and toxicokinetic evaluations of per- and polyfluoroalkyl substances (PFAS) for new approach method (NAM) application. **B. Wetmore**

11:15. Photodegradation of perfluorooctanoic acid by brookite and anatase titanium dioxide nanoparticles in acidic, neutral, and basic aqueous conditions. **L. Coward**, O. Love

11:35. Characterization and degradation of polyfluorinated substances. **E. Hayden**, J.C. Poler

Durham Arts Council
Duke Rehearsal Hall

Physical Chemistry: Theory Development and Experimental Frontiers

Cosponsored by PHYS
D. A. Canelas, *Organizer*
K. Lao, L. M. Thompson, *Presiding*

9:30 Opening Remarks.

9:35. Accelerating quantum chemistry calculations using Grassmannians. **K. Lao**

9:50. Time propagation of electronic wavefunctions using nonorthogonal determinant expansions. **L.M. Thompson**

10:05. Quantum algorithms for simulating quantum dynamics in the condensed phase environment. **F. Wang**, P. Walters

10:20 Break.

10:30. Magnetically-driven quantum phase transitions in a low-dimensional pyrazine-bridged Cu²⁺ chain magnet. **A. Blockmon**, K. Park, J. Jo, E. Kirkman-Davis, M.M. Turnbull, M. Lee, J. Singleton, S. McGill, H. Kim, J. Lee, J. Musfeldt

10:45. Atoms-in-molecules study of charge-shift bonding in neutral and protonated molecules RX and RXH⁺ (R=Me, Et, *i*-Pr, *t*-Bu; X=OH, NH₂, SH, PH₂, F, Cl). **D.A. Clabo**, J.N. McCutcheon

11:00. Quantum chemistry calculations of halogenated phenols. **S. Cerabona**, G.G. Brown

11:15 Break.

11:25. Computing tunneling paths with Hamilton-Jacobi equation within a classical wave front propagation method. **B.K. Dey**

11:40. Density-functional tight-binding parameter development for evaluating carbon nanoparticle stability in molten salts. **T. Walker**, S. Irle

Durham Convention Center
Junior Ballroom D2

Polymer Chemistry and Materials Science Research and Development

Cosponsored by PMSE and POLY
D. A. Canelas, *Organizer*

9:30 Opening Remarks.

9:35. Reinforced nanocomposites from aqueous polymer-graphene oxide nematic mixtures. **M. Hegde**, M.P. Bakas, J.M. Migliore, A.S. Kumbhar, E.T. Samulski, T.J. Dingemans

9:50. Self-crosslinkable thin film composites of carbon nanotube loaded PEI and single layer graphene. **O. Valenzuela**, G. Liu

10:05. Oxygen-doped antimonene monolayer as a promising anchoring material for lithium-sulfur batteries: A first-principles study. **V. Zhu**, X. Luo

10:20 Break.

10:30. Alignment of gold nanorods in shape-memory polymer films. **Z.A. Watts**, D.J. Sawyer, A.N. Simpson, M.H. Rizvi, T.N. Robinson, M.M. Ghelardini, A.L. Oldenburg, J.B. Tracy

10:45. Increasing the viscosity of a rodlike polyelectrolyte with a monovalent salt. **J. Migliore**, M. Hegde, Q. Tang, M. Rubinstein, T.J. Dingemans

11:00. 3D-printed hydrogels as photothermal actuators. **M.M. Ghelardini**, M. Geisler, N. Weigel, J. Hankwitz, N. Hauck, J. Schubert, A. Fery, J. Thiele, J.B. Tracy

11:15 Break.

11:25. Magnetic reprogramming of self-assembled hard-magnetic cilia. **M. Clary**, S.N. Cantu, J. Liu, B. Evans, J.B. Tracy

11:40. Cellulose acetate-Ti (IV) tungestomolybdate : A biopolymer supported nano composite exchanger for the removal of selected heavy metal ions from aqueous solution. **B.M. minase**

11:55. Structure-property relationships of thermosensitive polymeric lanthanide sequestrants. **S. Chittari**, M. Bogen, A. Knight

12:10. A computational approach to insights into aggregate formation between cellulose acetate and xylan acetate. **M. SHISHIR**, F. Rahmani, S. Park, T. Treasure, M.A. Pasquinelli, S.S. Kelley, S. Park

Durham Convention Center
Meeting Room 4

Roger M. Leblanc Symposium of Molecular and Nano Sciences

Cosponsored by BIOL, COLL and MEDI
Financially supported by MTSU
C. Wang, Y. Zheng, *Organizers*

9:30 Introduction of the symposium.

9:40. Bioorthogonally activated photoresponsive systems. **P. Kele**

9:55. pMAIRS: A novel method to address both conformation and orientation of α -helix in monolayer at interface. **C. Wang**

10:10. Evanescent scattering microscopy for label-free characterization of single proteins. **S. Wang**

10:25. Developments of photoswitchable fluorophores and spectroscopic single-molecule imaging methods toward functional super-resolution microscopy. **Y. Zhang**

10:40 Coffee break.

10:50. DNA-based supramolecular assemblies. **E. Skelly**, K. Afonin

11:05. Eliminating surface defects on CdSe NCs by Z-type ligand passivation. **J. Kelm** , J. Bost, Y. Kanai, J.L. Dempsey

11:20. Au nanoclusters stabilized on Ag@SiO₂@Au nanotriangle: Insights into FRET and synergistic effects with LSPR. **W.K. Evadzi**, U.M. Kuruppu, M.K. Gangishetty

11:35. Rationally designed RNA-DNA fibers and their biomedical applications. **Y. Radwan**, K. Afonin

Durham Convention Center
Junior Ballroom A1

Sharing Experiences and Building Capacity of LGBTQIA2S+ Chemists in the South

Cosponsored by D&I
S. Banerjee, J. Barnes, *Organizers*

10:00 Opening Remarks.

10:10. Alphabet soup to pride: The history of LGBTQ+ chemical professionals in the ACS. **C.J. Bannochie**

10:30. Paramagnetic rainbows: Synthesis of high-spin d⁵ fluorophores. **A.B. Scharf**

10:50. Mentoring chemistry/STEM students with intersectional identities: (Un)training ourselves. **S. Banerjee**

11:10 Panel Discussion.

Durham Convention Center
Grand Ballroom I

Biochemistry Research and Development Poster Session

Cosponsored by BIOL
D. A. Canelas, K. C. Glasgow, *Organizers*

11:10 - 1:10

101. Assessing the impact of buffer salt choice on the formation of DNA I-motifs [Poster Board #101]. **C. West**, L.A. Rolband, J. Krueger

102. Determining the mechanism of translocation of ClpA while unfolding polypeptide substrates [Poster Board #102]. **L. Islam**, A.L. Lucius

103. Roles of ionizable residues in proton channel activity through protein design [Poster Board #103]. **A. Rohrbach**, J. Lopez, H.T. Kratochvil

104. Metal cofactor replacement in the multifunctional catalytic enzyme Dehaloperoxidase [Poster Board #104]. **T. Vu**, R. Ghiladi

105. Investigating the diiron active site's role in nitric oxide peroxidase activity within the hemerythrin-like protein isolated from *M. kansasii* [Poster Board #105]. **S. Jennings**, J.D. Caranto, V.L. Davidson

106. Ferric superoxide intermediate initiates P450-catalyzed cyclic di-peptide dimerization [Poster Board #106]. **H. Gering**, X. Li, H. Tang, P. Swartz, W. Chang, T.M. Makris

107. Synthesis and evaluation of irreversible inhibitors against a key fungal enzyme [Poster Board #107]. C. Curran, J. Dietz, **C.J. Halkides**, L. Koellner, A. Koenig-Dummer, J. Parker, N. Simmons, R.E. Viola

108. Evaluation of the broad applicability of newly discovered E3 ligase recruitment strategies for targeted protein degradation [Poster Board #108]. **L. Mather**, L.I. James

109. Advancing lignin bioconversion: Structure-activity relationships of cytochrome P450 aromatic O-demethylase using QM-cluster models [Poster Board #109]. **T. Suhagia**, R. Hammati, Q. Cheng, N.J. Deyonker

110. Increased conversion of hypocrellins to Hypomycins under anaerobic growth conditions [Poster Board #110]. **R. AL-QIAM**, F. Tuglak Khan, M. Rangel-Grimaldo, H. Raja, C. Pearce, S. Hematian, N.H. Oberlies

111. Fluorination of Diepoxin- η : Characterization and anticancer activity evaluation of semisynthetic derivatives of spirobisnaphthalenes [Poster Board #111]. **H. Pourhadi**, T. El-Elimat, M. Rangel-Grimaldo, T. Graf, J. Falkinham, M. Khind, J. Burdette, C. Pearce, N.H. Oberlies

112. A design of experiment approach to evaluate extracellular vesicle stability and integrity in select buffer combinations for long-term storage [Poster Board #112]. **A. Kumari**, **F. Ebrahimi**, K. Dellinger

113. Profiling extracellular vesicles in N2a cells simulating tauopathy [Poster Board #113]. **S. Ghadami**, F. Ebrahimi, K. Dellinger

114. The characterization of freshwater fungi for antimicrobial studies [Poster Board #114]. **T. Cameron**, V. Anderson, C. Espinoza-Barrios, C. Laws, A. Shawkwat, H. Raja, T. Graf, N.B. Cech, N.H. Oberlies

115. Development of covalent antagonists and bivalent degraders to validate the biological role of M-phase phosphoprotein 8 (MPP8) [Poster Board #115]. **J.L. Sanchez**

Durham Convention Center
Grand Ballroom I

Inorganic Chemistry Research and Development Poster Session

Cosponsored by INOR

D. A. Canelas, K. C. Glasgow, J. M. Harrington, *Organizers*

11:10 - 1:10

116. Controlling the CO₂ reduction reaction through dual active sites embedded in expanded porphyrins: A DFT study [Poster Board #116]. **G. McCarver**, T. Yildirim, W. Zhou

117. Terpyridine ruthenium oxime complexes: Models for proton coupled electron transfer [Poster Board #117]. **E.T. Bell-Loncella**, C.S. Bean, A. Tukanowicz-Hassett

118. Neutral ternary complexes of BiI₃/CuI and SbI₃/CuI with tetrahydrothiophene [Poster Board #118]. **R.D. Pike**, J.H. Ballenger, D.A. Welch, A.D. Nicholas

119. Synthetic discovery of the first Sn(II)-perovskite oxides through flux-mediated ion-exchange techniques [Poster Board #119]. **E.A. Gabilondo**, S. O'Donnell, R. Broughton, R.J. Newell, J.L. Jones, P.A. Maggard

120. Imidazole thiones show metal-mediated DNA interactions [Poster Board #120]. **J. Alewine**, C. Goodman, J.L. Brumaghim

121. Cationic TM-Al TM = Cu, Ag, Au complexes for catalytic (de)hydrogenation [Poster Board #121]. **e. masaeli**, O. Garcia, M. Munoz

122. Circumventing barriers to metal hydride formation using ligand-cooperativity in proton-coupled electron transfer reactions [Poster Board #122]. **C. Montgomery**, M.Z. Ertem, L.H. Chevalier, J.L. Dempsey

123. Mechanistic investigations of a new class of copper dependent enzymes: BURP domain peptide cyclases [Poster Board #123]. **M. Noyon**, A. Buttar, F. Tuglak Khan, S. Lima, J.R. Chekan, S. Hematian

124. Chlorinated Triarylboranes: Leveraging steric bulk to expand borane catalysis [Poster Board #124]. **N. DeSousa**, M.R. Gagne

125. Altering the growing conditions of host crystals in the crystalline sponge method [Poster Board #125]. **E. Jackson**, T.R. Ramadhar

- 126.** Investigation of effect of hole doping on the magnetic and structural behavior of CaCo_2As_2 [Poster Board #126]. **S.A. Adegboyega**, M. Shatruk
- 127.** Investigation of magnetoelectric coupling in a mixed-valent Mn_4Na complex with trigonal-bipyramidal metal core [Poster Board #127]. **D.J. Mondal**, P. Wang, J. Wampler, V. Zapf, M. Shatruk
- 128.** ‘Ship-in-a-Bottle’ synthesis of metal phthalocyanines in zeolites [Poster Board #128]. **E. Wissman**, G.R. Rana, I. Ivanov, M.M. Bindu, **M.G. Bakker**
- 129.** Reactivity of 2,4-dichlorophenol in hemoglobin-dehaloperoxidase A & B [Poster Board #129]. **M. Aktar**, S. Franzen
- 130.** Exploring Fe(II) spin-crossover complexes for surface functionalization [Poster Board #130]. **D. Kumar**, M. Gakiya-Teruya, M. Shatruk
- 131.** Development of $\text{Si}(\text{pincer})_2$ complexes for organic and printable electronics [Poster Board #131]. **A. Adeyemi**, M. Cho, H. Smith, M. Sun, P. Ilies, W. Lomax, T.A. Schmedake
- 132.** Spectroscopic investigation of Ni (III) diethyldithiocarbamate during chemical oxidation from Ni (II) to Ni (IV) [Poster Board #132]. **R. Islam**, B. FARNUM
- 133.** Hydrothermal synthesis and crystal growth of novel transition metal vanadates [Poster Board #133]. **M. Foroughian**, C. McMillen, J.W. Kolis
- 134.** Using pendent proton donor relays and added base to control product selectivity during dioxygen reduction with MN complexes [Poster Board #134]. **E.N. Cook**, I.M. Courter, D.A. Dickie, C.W. Machan
- 135.** Study of manganese and copper assemblies for cooperative reactivity toward dioxygen in varying solvents [Poster Board #135]. **D.S. Porter**, F. Tuglak Khan, S. Hematian
- 136.** Immobilization of molecular catalysts on solid supports utilizing new motifs [Poster Board #136]. **J.J. Kuchta**, S. Moody, A.K. Vannucci
- 137.** Theoretical insights into nitrite reduction mechanisms catalyzed by Ni, Mn, and CrDIM electrocatalysts in aquatic media [Poster Board #137]. **E. Adu Fosu**, C. Worster, M. Ghosh, S.E. Braley, R. Ezhov, Y. Pushkar, J.M. Smith, E. Jakubikova
- 138.** Actinide-containing photochromic metal-organic frameworks [Poster Board #138]. **C.R. Martin**
- 139.** Electrochemical studies of solvent dependent speciation in copper(I) complexes [Poster Board #139]. **M. Tapia**, F. Tuglak Khan, S. Hematian

- 140.** Water splitting using VPI-100 (Cu) [Poster Board #140]. **C. Orlando**, B. Thomas, A.J. Morris
- 141.** Synthesis of samarium-containing magnetic nanoparticles [Poster Board #141]. **J. Maalouf**, D. Carnevale
- 142.** Changes in the magnetization of hexadecafluorinated iron phthalocyanine induced by modification from powder to nanowires [Poster Board #142]. **C. Metzler**, J. Cruz Lozada, R. Rosario, S. Flores Chalco, L. Fonseca, R. Clerac, D.M. Pinero Cruz
- 143.** Fundamental exploration of the effect of molecular reorganization on charge-separated state lifetimes [Poster Board #143]. **N.S. Abeynayake**, T. Cheng, A.J. Morris
- 144.** A rare bird: U^{+5} and U^{+6} in uranium sulfides [Poster Board #144]. **A. Berseneva**, H. zur Loye
- 145.** Binding chromium(III) to form mixed Cr(III),Fe(III) serum transferrins [Poster Board #145]. **D.R. Graham**, E. Drummond, M. Barrido, **J.B. Vincent**
- 146.** Extended structure lanthanide fluoride/silicates prepared using different synthetic routes [Poster Board #146]. **C. Ingram**, **A. Smith**, H. Herndon, A.T. Hines, N. Keerthisinghe, L.W. Masachchi, H. zur Loye
- 147.** Synthesis and comparative analysis of Fe_xNi_ySn magnetic nanoparticles [Poster Board #147]. **S. Celis**, D. Carnevale
- 148.** Synthesis of metal chalcogenide magnetic nanoparticles [Poster Board #148]. **D. Giordano**, D. Carnevale
- 149.** Comparison of nitrate reduction mechanisms in surface-conjugated and homogenous cobalt-based electrocatalysts [Poster Board #149]. **C. Worster**, M. Ghosh, S.E. Braley, R. Ezhov, Y. Pushkar, J.M. Smith, E. Jakubikova
- 150.** Comparisons of bpy and phen ligand backbones in Cr-mediated co-electrocatalytic CO_2 reduction [Poster Board #150]. **A.G. Reid**, M.E. Moberg, C. Koellner, S.L. Hooe, K.R. Baugh, D.A. Dickie, C.W. Machan
- 151.** Influence of synthetic temperature on surface states of $CuGaO_2$ [Poster Board #151]. **H. Yeasmin**, Z. Adams, B.H. Farnum
- 152.** Methodology development for orthogonal functionalization of molecular catalysts on silicon surfaces: Towards cascaded reactions for catalytic CO_2 reduction [Poster Board #152]. **A.R. Combs Bredar**, P. Fernandez, E. Stewart-Jones, J.M. Mayer, R. Lopez, J.L. Dempsey

153. Anticancer activity of ruthenium polypyridyl complexes: Soluble complex *versus* micro-, nano-particles [Poster Board #153]. **S.M. Kriger**, J. Laisney, D. Havrylyuk, J.M. Unrine, D.K. Heidary, P.C. Glazer

154. Synthesis of zwitterionic ruthenium and rhodium complexes incorporating aromatic N-heterocycles and group 13 metals [Poster Board #154]. **G. Sanchez Lecuona**, V. Montiel-Palma

155. Alkali metal modulation of the Ce^{3+/4+} couple [Poster Board #155]. **A.C. Boggiano**, C.M. Studvick, J. Bacsa, I.A. Popov, H.S. La Pierre

156. Mid-actinide Imidophosphorane complexes: Redox chemistry & reactivity [Poster Board #156]. **J. Niklas**, K.S. Otte, C.M. Studvick, A.C. Boggiano, J. Bacsa, I.A. Popov, H.S. La Pierre

WEDNESDAY AFTERNOON

Durham Convention Center
Junior Ballroom D3

Advanced Polymeric Nanocomposite Membranes for Water and Wastewater Treatment

Cosponsored by ENVR
J. C. Poler, *Organizer*
A. Sahu, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05. Functionalized cellulose as a nanocomposite membrane material for water purification. **C. Kwiatkowski**, E. Hayden, J.C. Poler

1:20. New reverse osmosis membranes for wastewater treatment. **M.D. Armstrong**, S. Mecham, J. Riffle

1:35. Effective adsorbent for GenX removal from water by decorating electrospun polyacrylonitrile nanofibers with Polyaniline. **I. Jahan**, L. Zhang

1:50. Advanced polymeric nanocomposite membranes for water and wastewater treatment. A. Sahu, R. Dosi, C. Kwiatkowski, S. Schmal, **J.C. Poler**

Durham Arts Council
Adaron Hall

Analytical Chemistry Research and Development

Cosponsored by ANYL
Z. S. Davis, G. E. Potts, *Organizers*
M. Bonizzoni, J. Mierzwa, *Presiding*

1:00 Introductory Remarks.

1:05. Chemical discrimination of multiple phenolic acids with a cyclodextrin supramolecular host. X. Yao, **M. Bonizzoni**

1:20. Applying process control to inform reproducibility in research. **K. Williamson**, I. Cocklereece, Z. Johnson, Y. Mo, D. Herr

1:35. Strategic cleavable sidechains for thermal stability in polymer solar cells. **J. Shanahan**, W. You

1:50. Characterization of multidirectional stationary phase gradient formation along commercial octyl functionalized HPLC columns. **T. Cecil**, S.C. Rutan, M.M. Collinson

2:05 Intermission.

2:15. Novel approach to method optimization for gas chromatography-mass spectrometry. **C.O. Granger**, S. Gamble, J.M. Mannion

2:30. Determination of some heavy metals in cat and dog nails by slurry sampling atomic absorption spectrometry (SS-AAS). **J. Mierzwa**

2:45. Quantitative interfacial affinity of sulfates in model marine aerosols. **J. Patterson**

Durham Arts Council
IBM Rehearsal Hall

Biochemistry Research and Development

Cosponsored by BIOT
D. A. Canelas, *Organizer*
B. Fuglestad, *Presiding*

1:00 Introductory Remarks.

1:05. Improved tools for exploration of structure, function, and inhibition at the protein-membrane interface. **B. Fuglestad**, A.J. Castillo, A.M. Develin, C.L. Labrecque, S.H. Walters

1:20. From lab to field: Engineered genetically-encoded biosensors for agriculturally-relevant macrolides detection. **N.E. Montero**, G.J. Williams

1:35. Characterization of antifungal peptoid dendrimers. **M.R. Johnson**, K. Bicker

1:50 Break.

2:00. Detecting and characterizing protonation-coupled conformational ensembles in microRNAs using pH-differential DMS-map and NMR. **E. Faison**, A. Nallathambi, Q. Zhang

2:15. Inhibition of SARS-CoV-2 RNA-dependent RNA polymerase enzymatic activity by antibiotics. **K. Gowda**, **V. Chaudhary**, P. Dinh, G. Dean, J. Wong, D.S. Lewis, V.V. Mody, S. Taval

2:30. Selective targeting and modulation of RNA G-quadruplexes in long noncoding RNA MALAT1 with small molecules. **J.G. Martyr**, M. Zafferani, M.D. Zorawski, N.I. Montalvan, D. Muralidharan, A.E. Hargrove

Durham Convention Center
Grand Ballroom I

Computational Chemistry: Educational Impact and Research Advances Poster Session

Cosponsored by CHED and COMP
D. A. Canelas, S. C. Sendlinger, *Organizers*

1:00 - 3:00

Poster Session.

101. Computational modeling of heterogeneous electron transfer: Elucidating double layer and polarization effects [Poster Board #101]. **C.A. Renfro**, J. McDaniel

102. Understanding radical scavenging mechanism involving phenoxy compounds by computational chemistry software [Poster Board #102]. **T. dey**

103. Computational electrosynthesis: Mechanistic study of an anodic coupling reaction between an electron-rich olefin and an alcohol [Poster Board #103]. **N. Khan**

104. Cyanobutadiene isomers of astrochemical significance: Computed negative ion photoelectron spectra and thermochemistry [Poster Board #104]. **J.A. Dupuy**, D.N. Koku Hannadige Abeysooriya, W.K. Gichuhi

105. Adsorption and activation of CO₂ on graphitic carbon nitride supported single-atom Al catalyst: A computational investigation [Poster Board #105]. **M. Wijesingha**, Y. Mo

Durham Convention Center
Junior Ballroom D2

Materials in Delivery Science

Cosponsored by BIOT, MEDI and POLY
M. Nurunnabi, *Organizer*

1:00 Opening Remarks.

1:05. Theranostic polymersomes in neuropathic lysosomal storage disease. D. Foster, A. Cakley, N. Shah, **J. Larsen**

1:25. Prodrug engineering for improved drug delivery and synergistic cancer therapy. **F. Zhang**

1:45. A photothermal driven chemotherapy for the treatment of metastatic melanoma. H. Bhatt, R. Diwan, **M. Nurunnabi**

2:05 Break.

2:15. Studying and fine-tuning cancer cell death pathways associated with photo-activated polysilsesquioxane nanoparticles. **J.L. Vivero**, H. Vadarevu

2:35. Modulating the antibacterial activity of photo-responsive nanoparticles via sequential light excitation mode. **V.S. Godakhindi**, J.L. Vivero

2:55. Porphyrin-based nanoparticles for the improvement of photodynamic therapy against cancer. **P. Anil Kumar Jeeja**, A. Nguyen, A. Eliasof, A. Berger, P. Loman-Cortes, J.L. Vivero

Durham Convention Center
Junior Ballroom A2

Organic Chemistry Research and Development

Cosponsored by ORGN
D. A. Canelas, *Organizer, Presiding*
R. El Mokadem, *Presiding*

1:00 Introductory Remarks.

1:05. Ketone-olefin coupling of aliphatic and aromatic carbonyls catalyzed by excited-state acridine radicals. N. Venditto, Y.S. Liang, **R. El Mokadem**, D.A. Nicewicz

1:20. Copper-mediated regioselective Boracarboxylation of unactivated alkenes. **C. Gordon,**
B.V. Popp

1:35. Highly acidic cyclopentadiene derivatives bearing Fluoroaromatic substituents. **H.**
Ramsey, P.A. Deck

1:50. Substrate-selective silylation of amino alcohols via macrocyclic catalysts. **A. Seilkop,** A.
Odoh, N. Coradi, J. Wright, B. Kim

2:05 Break.

2:15. Synthesis and self-assembling properties of photochromic carbohydrate derivatives. **G.**
Wang, P. Aryal, G. Grandhi

2:30. Alkoxy radical generation mediated by sulfoxide cation radicals. **D. Finis,** D.A. Nicewicz

2:45. Synthesis of conjugated electrophilic N6 adenine SAM analogs. **G. Harris,** L. Comstock

Durham Convention Center
Junior Ballroom C

Organic Chemistry Research and Development

Cosponsored by ORGN
D. A. Canelas, K. C. Glasgow, *Organizers*
A. A. Thomas, *Presiding*

1:00 Opening Remarks.

1:05. Breaking the tert-butyllithium contact ion pair: A gateway to alternate selectivity in
lithiation reactions. **A.A. Thomas**

1:20. Synthesis and characterization of fluorinated paramagnetic imidazolium-based ionic liquids
containing lanthanide anions. **J. Knoop,** J.R. Alston

1:35. C-H functionalization of thioethers. **K. Vargas,** J.M. Bray, S.G. Lewis, J.C. Meyers, J.M.
Buenavista, B. Dawitt, K.M. Lambert

1:50. C-H functionalization of bis(azolium) salts: Direct access to symmetrical and
unsymmetrical bis-abnormal CCC-NHC pincer complex precursors. **A. Cecil,** E. Fosu, T. Hollis

2:05 Break.

2:15. Breaking the *tert*-butyl lithium contact ion pair: A gateway to alternate selectivity in lithiation reaction. **J. Pina**, M. Crockett, A.R. Gogoi, R.F. Lalis, A.V. Nguyen, O. Gutierrez, A.A. Thomas

2:30. Predicting regiochemical outcomes of C-H borylations. **K.M. Lambert**

2:45. Functionalization of alkyl boronic esters. **M.D. Hamilton**, M. Kline, M. O'Reilly, B.V. Popp

3:00. Catalytic Hydroborylative intermolecular coupling of allenes for synthesis of highly substituted 1,3-diene compounds. **A. Abu Anzeh**

Durham Convention Center
Junior Ballroom A3

PFAS Compound

Cosponsored by ENVR

Financially supported by Nexus

W. Bodnar, A. Brennan, D. Macmillan, K. Renyer, *Organizers, Presiding*

1:00 Introduction.

1:05. Comparison of lists of per- and polyfluoroalkyl substances (PFAS) based on different definitions. **A.J. Williams**, L. Gaines

1:25. Exploring mobility trends in PFAS using SLIM high-resolution ion mobility-mass spectrometry (HRIM-MS). **T. Petti-Bacovin**

1:45. Development of a Python script to aid in identification of biotransformation products of emerging PFAS. **K. Renyer**, B. Payne, W.A. Willis, A. Brennan, D. Macmillan

2:05 Break.

2:15. Boron nitride materials for degradation of PFOA. **J.G. Clar**, A. Sheffield

2:35. Chemical characterization of per- and polyfluoroalkyl substances (PFAS) in North Carolina firehouses. **G.V. West**, C. Eichler, N. Chang, R.L. Turner, B.J. Turpin, J. Surratt

2:55 PFAS NEXUS Event.

Durham Convention Center
Meeting Room 3

Chemistry Education Research and Practice

Cosponsored by CHED
S. L. Johnson, *Organizer*

1:15 Introductory Remarks.

1:20. Effectiveness of a scholarship and enrichment program in improving recruitment, retention, and success of female students in STEM fields. **A.A. Carter, W. Powell, M. Pickering, J. Mcmillen, J. Hontz**

1:35. Surveying Florida's postsecondary educators on information literacy and associated threshold concepts. **M. Lam, K. Medina, C. Randles**

1:50. Why do we assess students? Exploring general chemistry instructors' knowledge about the purpose of assessment practices. **Y. Wang, L. Shi, J. Mitchell-Jones, M.N. Stains**

2:05. Student perspectives on remote learning in a large organic chemistry lecture course. **M. Castillo**

2:20 Break.

2:30. Unique online video e-book with video e-homework. **K. Trivedi**

2:45. Understanding student perceptions of specifications grading and its differential impact. **B.J. Yik, H. Machost, A. Streifer, M.S. Palmer, L. Morkowchuk, M.N. Stains**

3:00. Data science for Chemists: Integrating and evaluating the use of interactive digital python notebooks in a large enrollment undergraduate biochemistry course. **R. Brunk, K. Shukla, B. Hudson, M. Verber, B. Hogan, E.C. Brunk**

Durham Convention Center
Junior Ballroom D1

Environmental Engineering

Cosponsored by ENVR and I&EC
D. F. Call, L. Pal, *Organizers*

1:15 Opening Remarks.

1:20. Regeneration of zeolite nano resin (ZNR) for water treatment: Promising approach for enhanced contaminant removal. **R. Dosi**, D. Desai, J.C. Poler

1:35. Potable water; basic essential for life survival. **M. Omorogie**, B. Helmreich

1:50. Applying circular economy strategies to find solutions for SDG 12s: E-waste management case studies. **S. RIKITU**

2:05. Circular economy models for smart phones-a case of Taiwan. **S. RIKITU**

2:20 Break.

2:30. Skin effect continuum into equivalent circulating density in petroleum drilling. **K. Kanawi**

2:45. Skin effect power loss as encoded power for BPSK/QPSK communication. **K. Kanawi**

Durham Arts Council
PSI Theatre

Inorganic Chemistry Research and Development

Cosponsored by INOR

D. A. Canelas, J. M. Harrington, *Organizers*

B. Aguila, M. Johnson, *Presiding*

1:15 Introductory Remarks.

1:20. Kinetics of diopside reactivity for carbon mineralization in mafic–ultramafic rocks. **B. Aguila**, L. Hardee, Q. Miller

1:35. Reusable HNO sensor: Mechanistic origin of high reactivity and favorable conformation changes and potential improvements. J. Chu, D. Baizhigitova, V. Nguyen, **Y. Zhang**

1:50. Silica supported niobium sites tailored for selective olefin conversion. **R. Johnson**, K. Searles

2:05 Break.

2:15. Investigation of heterometal substitution in polyoxometalate-porphyrin hybrid materials for efficient charge transfer. **L. Hanna**, K. McDonald

2:30. Coordination chemistry of N-heterocyclic chalcogenones derived from caffeine. **M.J. Zelada-Bazán**, D. Rabinovich

2:45. Metal-catalyzed oxidation of peptides: Unraveling the reactivity of the *bis*-His site in Histatin-5. **L.J. Bontreger**, A.D. Gallo, K.J. Franz

3:00. Design, analysis, and application of pyrrole-based phosphine ligands. **M. Johnson**

Durham Convention Center
Grand Ballroom I

Methods and Applications of High-Resolution Mass Spectrometry Poster Session

Cosponsored by ANYL and ENVR
J. P. McCord, E. M. Ulrich, *Organizers*

1:15 - 3:15

Break.

101. Multi-year investigation of urban algal blooms in northwest Florida using LC-MS/MS [Poster Board #101]. **C. Kapczynski**

102. Evaluation of digestive transformation of *Withania somnifera* (Ashwagandha) plant extracts and bioactive compounds via UPLC-MS and untargeted metabolomics [Poster Board #102]. **S. Barr**, R.T. Williamson, W.K. Strangman

103. System suitability testing (SST) for mass spectrometry imaging (MSI): A machine learning approach [Poster Board #103]. **R. Kibbe**, A. Sohn, O. Dioli, E. Hector, D.C. Muddiman

104. Innovative sampling strategies for mass spectrometry imaging of *artemisia annua* leaf tissue by IR-MALDESI [Poster Board #104]. **Q. Mills**, S. Ashbacher, A. Sohn, D.C. Muddiman

105. Synthesis-based approach to elucidating metabolites of the gut-brain axis [Poster Board #105]. **K. Cahannell**

106. Exploring diet-derived metabolism via reverse-metabolomics [Poster Board #106]. **L.E. Sandusky**, E.C. Gentry

107. Identifying antimicrobial peptides from *Momordica charantia* using PepSAVI-MS [Poster Board #107]. **M. Hnilica**, L. Hicks

Durham Convention Center
Grand Ballroom I

Polymer Chemistry and Materials Science Research and Development Poster Session

Cosponsored by PMSE and POLY

D. A. Canelas, *Organizer*

1:15 - 3:15

Poster Session.

108. Gold nanoparticles conjugated with iodinated copolymers as a potential dual X-ray imaging contrast agent [Poster Board #108]. **A. Drakes**, P. He

109. Architectural expansion of a library of biohybrid block copolymers [Poster Board #109]. **K. Ready**

110. Polycarbodiimide removes textile dyes from aqueous solution [Poster Board #110]. **M. Lord**, J. Budhathoki-Uprety

111. Advancing pH detection in biofluids with single-walled carbon nanotube-based optical probes [Poster Board #111]. **N. Sultana**

112. Elucidating design rules for protein mimetic metalloenzymes [Poster Board #112]. **N. Calzadilla**, A. Knight, B. Allen

113. Photophysical studies of MOF encapsulated ruthenium polyimines for light activated drug delivery [Poster Board #113]. **M.N. Senn**, R.W. Larsen

114. Probing lignin and carbohydrate structural changes of various hardwood species throughout the Kraft pulping process [Poster Board #114]. **C.L. Burke**

115. Phenothiazine-based polyaniline derivative: Effects of side-chain, solvent, and dopant on the conductivity [Poster Board #115]. **H. Giri**, C. Scott

116. Synthesis and characterization of naphthalenediimine based copolymers [Poster Board #116]. **D. Argi**, T. Muthumali, R.C. Chiechi

117. Measuring epoxy cure kinetics using single-sided nuclear magnetic resonance [Poster Board #117]. **O. Cassara**, K. Copeman, J. Ballenger, S.J. Tate, C. Thompson, K. Sutterfield, S. Wood, T.K. Meldrum

118. Comparison of low and high molecular weight nitric oxide-releasing hyaluronic acid for corneal wound healing [Poster Board #118]. **M.E. Purvis**, M. Schoenfish

119. Expanding the scope of RAFT step-growth [Poster Board #119]. **S. Clouthier**, J. Tanaka, W. You

- 120.** Polymer modifications to optimize nanosensor output for analyte detection [Poster Board #120]. **S.M. Abello**, H. Dewey, J. Budhathoki-Uprety
- 121.** Quantitative structure-property relationship study of metal-organic framework bandgap [Poster Board #121]. **K. Williamson**, D. Herr, Y. Mo
- 122.** Aqueous synthesis of polyelectrolytes (ionomers) using non-metal based reducing agents [Poster Board #122]. **D. Desai**, J.C. Poler
- 123.** Influencing self-assembly of oligomeric peptide-polymer amphiphiles by changing monomer architecture [Poster Board #123]. **B. Allen**, N. Calzadilla, A. Gringeri, A. Knight
- 124.** Use of self-assembled monolayers to surface-initiate polymerization of poly(3-hexylthiophene) onto various surfaces [Poster Board #124]. **R. Augustine**, B. Augustine, P. Lundin
- 125.** Stereolithography of ionic liquids using a commercial 3D printer [Poster Board #125]. **e. riglioni**
- 126.** Development of optical nanosensors for the detection of quaternary ammonium compounds [Poster Board #126]. **H. Dewey**, N. Sultana, J. Budhathoki-Uprety
- 127.** Isomer and molecular weight effects on polyetherimide coatings for corrosion protection of aluminum alloys [Poster Board #127]. **T. Sill**, C. Larriuz, V. Ponce Valderrama, P. Johnson, H. Castaneda, S. Banerjee
- 128.** Versatile polymeric chelators for rare earth element isolation [Poster Board #128]. **E. Barkley**, M. Bogen, A. Knight
- 129.** Connecting polymer dynamics to the sequestration of water contaminants [Poster Board #129]. **S.F. Grizzard**, P. Dykeman-Birmingham, M. Bogen, A. Knight
- 130.** Photophysical comparison between Tetra-N-Methyl-Pyridyl Porphyrin (TMPyP) and Meso-tetra(4-N,N,N-trimethylanilinium) porphyrin (4TANP) [Poster Board #130]. **Q. Maqbool**, R.W. Larsen
- 131.** Developing ester-incorporated monomers to enable the degradability and recyclability of organic semiconductors [Poster Board #131]. **A. Megret Bonilla**, J. Neu, W. You
- 132.** Comparative study between synthesis efficiency of hydroxyl-terminated polybutadiene using ruthenium catalysts [Poster Board #132]. G.A. Su, **P. Reiter**, M.D. Schulz
- 133.** Sodium alginate-based ink for 3D printing of dosage to deliver pharmaceutical drug [Poster Board #133]. **F.K. Rony**, G. Kimbell, D. Clay, M. Azad

134. Photophysical studies of ligand photorelease associated with ruthenium-based complexes encapsulated within polyhedral zinc metal organic frameworks [Poster Board #134]. **D. Sellers**, R.W. Larsen

135. Optimizing dendrimer-peptide synthesis using a model system [Poster Board #135]. **J. Linville**, J. O'Brien, C.B. Gorman

136. Leveraging specific DNA hybridization to assemble diverse block copolymers [Poster Board #136]. **K. Coghlan**, K. Ready, A. Knight

137. Epoxidized cottonseed oil as a potential additive for waterproof packaging [Poster Board #137]. **L. Meza Carvajal**, L. Chacon, N. LAVOINE, R. Venditti

138. Synthesis and characterization of ion-imprinted polymers for selective lanthanide separation [Poster Board #138]. **D.N. Smith**

139. Optimizing design of polymer binders for rare earth element isolation [Poster Board #139]. **M. Bogen**, S. Chittari, E. Barkley, A. Knight

140. Inhibiting norovirus infections via modular hyperbranched polymers with terminal glycan moieties [Poster Board #140]. **J. Mase**, N. Lidman, S. Newman, J. Rubino, M.D. Schulz

141. Withdrawn

142. Synthesis of polymer-nucleobase composites for chemotherapy drug capture [Poster Board #142]. G. Su, **H.S. Muller**, M.D. Schulz

Durham Convention Center
Meeting Room 4

Roger M. Leblanc Symposium of Molecular and Nano Sciences

Cosponsored by BIOL, COLL and MEDI

C. Wang, Y. Zheng, *Organizers*

P. Kele, S. Wang, *Presiding*

1:15. Effect of asymmetric nanostructuring on nanomotor behavior in actuating fields. **S. Ahmed**, T. Afsari, C. Weissing

1:30. Correlation of saccharide carbon dot graphene defect density with dopamine electrochemical sensitivity. **R.C. Nepal**, C.C. Chusuei

1:45. Elucidating the key parameters of nucleic acid nanoparticles that allow for RIG-I activation. **L. Danai**

2:00. Metal organic frameworks functionalized with Cr(III) metal complexes for selective oligomerization of ethylene. **V. Yempally**, H. Zhou, S. Madrahimov

2:15 Coffee break.

2:25. Observing the dissolution of anisotropic ruthenium dioxide nanowires under anodic conditions via graphene liquid cell transmission electron microscopy. **S.A. Vigil**, I.A. Moreno-Hernandez

2:40. Electrically driven yellow light emission from phase-pure 1D CsCu₂I₃ metal-halides. **U.M. Kuruppu**, M.K. Gangishetty

2:55. Cationic carbon dots and their application in cancer cells inhibition as well as gene delivery. **J. Chen**, R.M. Leblanc

3:10 Remarks on the symposium by Professor Roger M. Leblanc.

Durham Arts Council
Duke Rehearsal Hall

Physical Chemistry: Theory Development and Experimental Frontiers

Cosponsored by PHYS
D. A. Canelas, *Organizer*
K. Lao, S. Nkomo, *Presiding*

1:30 Introductory Remarks.

1:35. Understanding the origins of complex oscillations of coupled Belousov-Zhabotinsky chemical oscillators. **S. Nkomo**

1:50. Predicting the reactions of CS₂, OCS, and CO₂ with group IV and group VI transition metal oxides. **M.S. Blair**, Z. Lee, D.A. Dixon

2:05. Rigorous and reproducible computational enzymology: The Rinrus software toolkit. **N.J. Deyonker**

2:20. Dependence of redox hopping charge transfer on carrier species in MOFs. **m. Yan**, Z. Bowman, A.J. Morris

Durham Convention Center
Junior Ballroom B

Shining a Light on Synthetic Fuels

Cosponsored by ENFL

D. Kurtz, A. J. Miller, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40. Covalent and non-covalent strategies for constructing hybrid photoelectrodes for light-driven reduction of carbon dioxide. **J.L. Dempsey**, B. Huffman, G.P. Bein, A. Jordan, R. Powers, R.N. Sampaio, S.J. Tereniak, M. Stewart, X. Jia, N. Hazari, A.J. Miller, C.L. Donley

2:00 Speaker 1 Q&A.

2:05. Photocatalytic CO₂ reduction with a nickel complex supported by a redox-active pentadentate ligand featuring intramolecular H-bonding interactions. Z.H. Turner, J. Ferdous, A. Antony, **J.W. Jurss**

2:25 Speaker 2 Q&A.

2:30. Nickel(II) and Cobalt(I) pincer complexes for reduction of CO₂. **E.T. Papish**, W. Yao, S.Y. Manafe

2:50 Speaker 3 Q&A.

WEDNESDAY EVENING

Durham Convention Center
Grand Ballroom I

Chemistry Education Research and Practice Poster Session

Cosponsored by CHED

S. L. Johnson, *Organizer*

5:00 - 7:00

101. Holistic student support integrated in the chemistry major experience: Longitudinal impact on student engagement and retention [Poster Board #101]. **S.A. Wasileski**, J.M. Schmeltzer, A.L. Wolfe

102. Characterization of a putative low molecular weight protein tyrosine phosphatase (LMW-PTP) from octopus: A course-based undergraduate research experience (CURE) [Poster Board #102]. **D.F. McCain**, E. Funkhouser, E. Bello, A. Mon, V. Townsend

103. Organic chemistry students' representational competence skills in the context of chair conformations [Poster Board #103]. **F. Rotich**, L. Wright Ward, C. Beck, M. Popova

104. Development of "chemistry first day" to increase recruitment at UNC Asheville [Poster Board #104]. **A.L. Wolfe**, S.A. Wasileski

105. Exploring student reasoning when translating between dash-wedge diagrams and chair conformations [Poster Board #105]. **Z. Bunch**, A. Jones, L. Wright Ward, M. Popova

106. Characterizing instructional practice and pedagogical reasoning related to teaching symmetry in inorganic chemistry courses [Poster Board #106]. **S. Hilborn**, L. Shi, Z. Edmonson, S. Pazicni, M. Popova

Durham Convention Center
Grand Ballroom I

Childhood Environmental Exposure/Toxicology Poster Session

Cosponsored by ENVR
W. Bodnar, K. C. Glasgow, *Organizers*

5:00 - 7:00

107. Investigating the impact of tire rubble microplastics sourced from recycling facilities dosed onto human epithelial lung carcinoma cells [Poster Board #107]. **Z. Eastman**, L. Rios-Colon, I. Walker Karega

108. Differential effects of primary-sourced synthesized polyethylene (PE) and secondary-sourced shredded high-density polyethylene (HDPE) microplastic leachate in A549 human epithelial lung carcinoma cells [Poster Board #108]. **L. Rios-Colon**, Z. Eastman, I. Walker-Franklin

Durham Convention Center
Grand Ballroom I

Coordination Chemistry, Synthesis, Characterization and Reactions Poster Session

Cosponsored by CATL, CHED, INOR, ORGN and PROF
Financially supported by Coastal Georgia Local Section
W. E. Lynch, *Organizer*

5:00 - 7:00

Poster Session.

109. Polydentate bis(amidine) ligands as molecular scaffolds for intertwined luminescent copper(I) clusters [Poster Board #109]. **K. Dowling**, C. McMillen, **M. Stollenz**

110. Synthesis and characterization of zinc dipyrin photosensitizers [Poster Board #110]. **J. SANZA**, C. McCusker

111. Redox properties and reactivity of nanocages with cobalt-porphyrin walls [Poster Board #111]. **P.T. Blackburn**, M. Lipke

112. Electronically delocalized Metalloviologens for applications in electrocatalysis and electronic materials [Poster Board #112]. **I.F. Mansoor**, B. Kessler, D. Wozniak, M. Lipke

Durham Convention Center
Grand Ballroom I

Green Chemistry-Driven Fundamental Research & Development of Nanocelluloses Poster Session

Cosponsored by CELL
L. A. Lucia, L. Pal, *Organizers*

5:00 - 7:00

113. Influence of various drying techniques on the adsorption characteristics of bacterial cellulose towards Methylene Blue in aqueous environments [Poster Board #113]. **Z. Hu**, L.A. Lucia, W.E. Krause

114. Analyzing the environmental impact of a commercial aquaponic system in Taiwan using LCA [Poster Board #114]. **S. RIKITU**

115. Conversion of cellulose to hexane using hydrogen bronze materials [Poster Board #115]. **M. Osman**, D.W. Scott

116. Understanding chiral nematic structure formation in cellulose nanocrystal suspensions: Impact of size and surface charge [Poster Board #116]. **S. Hong**, L.A. Lucia, N. LAVOINE

117. Regenerated biopolymer composites from ionogels for applications in 3D cell cultures [Poster Board #117]. **E. McDowell**, L. Fernandez, L.D. Yoder, B. Sadiku, K. Dellinger, J.R. Alston

118. Time-resolved analysis of synthesis and water uptake in 1-Butyl-3-Methylimidazolium Chloride (BmImCl) [Poster Board #118]. **L. Yoder**, J. Knoop, S.K. Hutchison, J.R. Alston

Durham Convention Center
Grand Ballroom I

PFAS Compound Poster Session

W. Bodnar, *Organizer*

5:00 - 7:00

119. Exploring the solvation process of perfluorooctanoic acid: One water at a time [Poster Board #119]. **H. Virkus**, A. Gracia, K. Murillo, J. Canales, W. Lin

120. Computational study of the thermal degradation reaction rate coefficients of perfluoroalkyl carboxylic acids [Poster Board #120]. **C. Paultre**, A.M. Mebel, K.E. O'Shea

121. Internal dose and in-life results after short term exposure of rats to short-chain PFAS [Poster Board #121]. **J. Bounds**, K. Renyer, D. Macmillan

122. Development of a targeted analytical method for measuring low level PFAS in serum [Poster Board #122]. **E. Thorp**, W. Bodnar, C. Liyanapatirana, K. Amato, K.E. Levine

Durham Convention Center
Grand Ballroom I

Shining a Light on Synthetic Fuels Poster Session

Cosponsored by ENFL
D. Kurtz, A. J. Miller, *Organizers*

5:00 - 7:00

135. Ground and excited state electronic structure of Fe(II), Ru(II) and Co(III) polypyridine complexes [Poster Board #135]. **M. Al Rammal**, E. Jakubikova

136. Rhenium *bis*-diimine catalysts for CO₂ reduction to formate [Poster Board #136]. **R.T. Alameh**, E. Asempa, C. Gillis, E.A. Assaf, H. Atallah, N. Durand, A.J. Miller, E. Jakubikova, F.N. Castellano

137. Diazafluorenone ligated Cp*Ir^{III} complexes: Leveraging hemilability to unlock new reactivity [Poster Board #137]. **E. Asempa**, M. Maenaga, E. Cueny, K. Goldberg, E. Jakubikova

- 138.** Understanding the photovoltage source of Si/MO_x coated photoelectrodes [Poster Board #138]. **A.R. Combs Bredar**, B. Shang, H. Nedzbala, J.M. Mayer, H. Wang, J.L. Dempsey
- 139.** Computational studies of electrocatalytic CO₂ reduction on a copper coordinated poly(triazine imide) [Poster Board #139]. **M. Deegbey**, M. Pauly, E. Adu Fosu, P.A. Maggard, E. Jakubikova
- 140.** Investigating the effect of steric hindrance in a new family of rhenium complexes bearing mono and bis diimine ligands [Poster Board #140]. **N. Durand**, R.T. Alameh, F.N. Castellano
- 141.** Non-covalent interactions of pincer ligands for switchable and tunable nickel catalysis [Poster Board #141]. **E.Z. Huebsch**, S. Acosta-Calle, C. Chen, A.J. Miller
- 142.** Hydrogen atom transfer promoted by visible light to form weak chemical bonds [Poster Board #142]. **T. Jurado**, B. Stratakes, A.J. Miller
- 143.** Designing multijunction silicon nanowires for solar-to-hydrogen conversion [Poster Board #143]. **S. Litvin**, T.S. Teitsworth, S. Bottum, J. Cahoon
- 144.** Synthesis and atomically-precise structure of a CU-coordinated carbon nitride and its catalytic reduction of carbon dioxide [Poster Board #144]. M. Pauly, M. Deegbey, L. Keller, S. McGuigan, G. Dianat, J. Wong, C. Murphey, B. Shang, H. Wang, J. Cahoon, R.N. Sampaio, Y. Kanai, G. Parsons, E. Jakubikova, **P.A. Maggard**
- 145.** Control of cage escape yields through steric bulk in transition metal complex photoredox reactions [Poster Board #145]. **J.S. McCarthy**, Q. Loague, G.J. Meyer
- 146.** Circumventing kinetic barriers to metal hydride formation in proton-coupled electron transfer reactions: What is the role of reorganization energy? [Poster Board #146]. **A.B. McCullough**, J. Amtawong, Y. Lam, M. Ford, J.L. Dempsey
- 147.** Discovery and investigation of a hybrid system for photocatalytic CO₂ reduction [Poster Board #147]. **S. McGuigan**, S.J. Tereniak, C.L. Donley, A. Smith, S. Jeon, F. Zhao, R.N. Sampaio, M. Pauly, L. Keller, L. Collins, G. Parsons, T. Lian, E. Stach, P.A. Maggard
- 148.** Noncovalent attachment of ruthenium-based molecular catalyst to silicon surfaces for photoelectrochemical CO₂ reduction [Poster Board #148]. **R. Powers**, A. Jordan, E.A. Assaf, X. Jia, S.J. Tereniak, R.N. Sampaio, N. Hazari, A.J. Miller, J.L. Dempsey
- 149.** Unlocking new pathways for photoelectrocatalytic solar fuels synthesis with an immobilized iridium complex [Poster Board #149]. **E. Reynolds**, D. Bass, A.J. Miller
- 150.** Progress towards photoelectrochemical molecular CO₂ to methanol cascade [Poster Board #150]. **A.M. Smith**, J.T. Sirlin, A. Muller, R.N. Sampaio, S. Ahmad, M.Z. Ertem, J.J. Concepcion, G.J. Meyer, A.J. Miller

151. Optimizing catalyst-semiconductor integration in hybrid photoelectrodes for light-driven CO₂ reduction [Poster Board #151]. **M.A. Stewart**, G.P. Bein, X. Jia, C. Dones Lassalle, R. Powers, N. Hazari, J.L. Dempsey

152. Electrografted multilayer catalysts films on silicon photoelectrodes for CO₂ reduction [Poster Board #152]. **T.S. Teitsworth**, L. Rotundo, G.P. Bein, R.N. Sampaio, C.L. Donley, J.L. Dempsey, G. Manbeck, M. Lockett

153. Chase's molecular synthesis facility: Soaking up the sun to turn down the heat [Poster Board #153]. **S.J. Tereniak**, B. Butler

154. Investigating iridium complexes with carbene ligands as catalysts in carbon dioxide reduction cascades [Poster Board #154]. **B. Travis**, S. Fernandez, A.J. Miller

Durham Convention Center
Grand Ballroom I

Ultrafast and Nonlinear Spectroscopy Poster Session

Cosponsored by ANYL

Financially supported by Light Conversion, Ultrafast Systems, and Phase Tech Spectroscopy
E. Ghadiri, T. Lian, L. Wang, *Organizers*

5:00 - 7:00

123. Hollow core fiber-based pulse compression for use in time-resolved photoelectron spectroscopy experiments [Poster Board #123]. **R. Barco**, Y. Qu, S. Ullrich

124. Ultrafast photochemistry of melanin and organic-inorganic melanin-based heterostructures using modern ultrafast pump-probe spectroscopy [Poster Board #124]. **F. Nourigheimasi**, L. Getter, R. Huo, E. Ghadiri

125. Ultrafast spectroscopy of chalcogenide nanoparticles for solar energy conversion applications [Poster Board #125]. **M. Sharif**, E. Ghadiri

126. Room-temperature superfluorescence in hybrid perovskite and its origins [Poster Board #126]. **M. Biliroglu**, G. Findik, J. mendes, D. Seyitliyev, L. Lei, Q. Dong, y. Mehta, v. temnov, F. So, K. Gundogdu

127. Signal deconvolution in 2D IR spectroscopy: Leveraging blind source separation for the feature extraction of congested protein signals [Poster Board #127]. **D. Boutwell**, J. Snyder, L.E. Buchanan

- 128.** Electronic relaxation dynamics of 6-Azauracil: The effect of ring-substitution on intersystem crossing [Poster Board #128]. **M. chudali**, S. Ullrich
- 129.** Monitoring the effect of lysine acetylation on amyloid beta fibrillation via 2DIR [Poster Board #129]. **C. Rohler**, L.E. Buchanan
- 130.** A high-speed phase-modulator for long-delay, coherent spectroscopy [Poster Board #130]. **B. Manna**, M.A. Berg
- 131.** Measuring carrier diffusion in MAPbI₃ photovoltaic cells with photocurrent-detected transient grating spectroscopy [Poster Board #131]. **Z. Gan**, Z. OUYANG, L. Yan, W. You, A.M. Moran
- 132.** Ultrafast 2D IR spectroscopy for the elucidation of the effect of nanoparticles on human islet amyloid polypeptide aggregation pathways [Poster Board #132]. **J. Snyder**, L.E. Buchanan
- 133.** Probing polarons dynamics in a ProDOT-co-EDOT polymer film using ultrafast spectroscopy [Poster Board #133]. **A. Umar**, A.L. Dorris, C. Grieco
- 134.** Ultrafast transient absorption spectroscopy of hydrocarbon radicals [Poster Board #134]. **J. Zhan**, N.D. Cooper, M.A. Reber

THURSDAY MORNING

Durham Convention Center
Junior Ballroom B

Southeastern Magnetic Resonance Conference (SEMRC)

Cosponsored by PHYS
A. I. Smirnov, M. A. Ter Horst, *Organizers*

8:30 SEMRC Welcome, Plenary Speaker Introduction.

8:35. Investigations of amyloid peptide aggregation, protein folding, and related processes by millisecond time-resolved solid state NMR. **R. Tycko**, C.B. Wilson, J. Jeon

9:20 Q&A with Dr. Tycko.

9:30. Translating fragment based screening technologies to natural product drug discovery. **R.T. Williamson**, C. Agee, W.K. Strangman, M.J. Recchia

9:50 Q&A with Dr. Williamson.

10:00. Non-targeted chemical analysis of consumer botanical products labelled as blue cohosh (*caulophyllum thalictroides*), goldenseal (*hydrastis canadensis*), or yohimbe bark (*pausinystalia johimbe*) by NMR and MS. G. Quiroz, C. Rider, S. Ferguson, A. Jarmusch, **G. Mueller**

10:15. Bringing NMR to chemical processes: Analyses of production samples with benchtop NMR. **R. Blough, A. Le-McClain, H. Robert**

10:30 Break, Introduction to NMR:Health and Environment.

10:40. In-situ ³¹P NMR study of adsorption and decontamination chemistry of gas-phase dimethyl phosphonate in MOF-808 and NU-1000. **M. Kasule**

10:55. Investigating the use of NOE-determined rotational correlation time for the characterization of nanoparticles through interactions with potential small molecule-based chemosensors. **V. Lin, L. Casabianca**

11:10. Varying the lipid composition of peptoid-based macrodiscs for oriented-sample NMR studies of membrane proteins. **A.R. Galiakhmetov, A. Shah, A. Lane, C. Davern, C. Proulx, A. Nevzorov**

11:25. Mixed, non-classical behavior in a classic allosteric protein. **P.J. Sapienza, J.P. Bonin, D.H. Jinasena, K. Li, H. Dieckhaus, K. Popov, J. Aube, A. Lee**

11:40. Bend it, twist it, squeeze it, stretch it: Comparing conformer generation packages and NMR restraints for macrocycle conformation determination. **E.B. Crull, A. Navarro-Vázquez, A.N. Jain, A.E. Jain, L. Gil, R.T. Williamson**

Durham Convention Center
Grand Ballroom I

Organic Chemistry Research and Development Poster Session

Cosponsored by ORGN
D. A. Canelas, K. C. Glasgow, *Organizers*

9:00 - 11:00

Poster Session.

101. Therapeutic modalities at Merck [Poster Board #101]. **J.L. Hanisak**

102. A microwave-assisted, two-step synthesis of indolo[3,2-c]quinolines via Fisher indolization and oxidative aromatization [Poster Board #102]. **S. Kiren**

103. Synthesis of *n*-fused polycyclic indole derivatives via Ru(II)-catalyzed C–H bond activation and intramolecular hydroarylation [Poster Board #103]. **N. Udayanga**

104. Determination and quantification of compounds in seeds of various herbs [Poster Board #104]. **H.V. Clontz**, C. Lagroon

105. New 4-methyl-N-(arylmethylene)-1-piperazinamines against tuberculosis [Poster Board #105]. **M.J. Hearn**, M.H. Cynamon, K. Anthony, S. Timalsina

106. Chiral Brønsted acid catalyzed cascade alcohol deprotection and enantioselective cyclization [Poster Board #106]. **J. Frost**, K.S. Petersen

107. Synthesis of 4,5-dihydro-1H-pyrazole derivatives as BRAF inhibitors [Poster Board #107]. **H. Bendure**, T. Grattan

108. Withdrawn

109. Asymmetric methodologies: Enantioselective synthesis of benzo-fused δ -lactams [Poster Board #109]. **A.H. Horchar**, K.S. Petersen

110. Toward an enantioselective preparation of diazacyclobutene atropisomers [Poster Board #110]. **M. Noori**, B. Miller, M. Maday, B. Borhan, D.C. Whitehead

111. Synthesis of alkyl fluorides and fluorinated unnatural amino acids via photochemical decarboxylation of α -fluorinated carboxylic acids [Poster Board #111]. **A. Gutierrez Bonet**, W. Liu

112. Protection and de-protection of boronic acids with diboron reagents [Poster Board #112]. **I. Khan**, K. Marichev

113. Benzothioxoquinazolinone-based inhibitors of the *mycobacterium tuberculosis* phosphopantethenyl transferase PPTT [Poster Board #113]. **L. Zwerneman**, X. Zhang, J. Aube, A. Singh, B. Gold, J. Zhang, N. Fotouhi, T. Kaneko, C.F. Nathan

114. Regioselectivity investigations of the internal base-directed aromatic Claisen rearrangement [Poster Board #114]. D. Tanas, **R. Li**, M.P. Croatt

115. Synthesis and application of a thiophene-based *o*-nitrobenzyl photolabile protective group for the synthesis of hydroxamic acids [Poster Board #115]. **A. Campbell Jr.**, C. Saint-Louis

116. Molecular design and synthesis of a visible light-absorbing thiophene-based *o*-nitrobenzyl photolabile protecting group for the synthesis of hydroxamic acids [Poster Board #116]. **O. Adjei-Sah**, C. Saint-Louis

- 117.** Stereoselective approach to the synthesis of the torreyunlignans [Poster Board #117]. **W.H. Kessler**, R.L. Carothers, B. Kropff, Z. Collins, W. Flannery, J.M. Carney
- 118.** Three-component, copper-catalyzed 1,4-aminoetherification of 1,3-dienes [Poster Board #118]. **M. Velopolcek**
- 119.** Enantioselective tandem deprotection-cyclization of alcohols to form lactones [Poster Board #119]. **S. Korb**
- 120.** Copper-catalyzed 1,3-aminocyclization of cyclopropanes as a rapid entry to γ -amino heterocycles [Poster Board #120]. **A. Nguyen**, J. Zhang, Q. Wang
- 121.** Synthesis & biological evaluation of 2,3-pyrrolidinediones [Poster Board #121]. **S.R. Kalliat**, J.G. Pierce
- 122.** BINOL phosphate a photochemical protecting group [Poster Board #122]. **K. Roach**, J. Olson
- 123.** Reactions of nitroxyl (HNO) with thioureas [Poster Board #123]. **M. Mahanes**, A. Negrellos, S.B. King
- 124.** Targeting the mRNA thiamine pyrophosphate riboswitch with small molecules [Poster Board #124]. A.M. Armaly, s. jin, **R. Sherrier**, **A.B. Wood**, J. Aube, K.M. Weeks
- 125.** Characterizing micelles through spectroscopy and the synthesis of arachidonic ethanolamide [Poster Board #125]. **E. Fisher**, C. Burns
- 126.** Development of regioselective asymmetric reductive coupling reactions of allenamides to access heteroatom-rich organic compounds [Poster Board #126]. **S. Collins**
- 127.** Investigation of optical, electronic and magnetic behavior of new class of Aza-BODIPY-based molecules [Poster Board #127]. **M.T. Oyelowo**, J. Schaffner, D.A. Blank, C.J. Ziegler, V. Nemykin
- 128.** Expedient synthesis of Tetrahydrobenzazepinones via formal [1,5]-rearrangement of cyclopropanone hemiaminals [Poster Board #128]. **Z.R. Ferrin**, V. Lindsay
- 129.** Synthesis of *N*-Aryl Peptides: Comparing the efficiency of Pd-catalyzed *N*-arylations and nucleophilic aromatic substitutions [Poster Board #129]. **K. McKinney**, H. Young, E.J. Warner, M. Broderick, C. Proulx
- 130.** Efforts in synthesis of daucane-type natural products with antiausterity activity against the PANC-1 pancreatic cancer cells [Poster Board #130]. **Y. Zhao**, I. Shin, E. Wang, H. Kim, J. Hong

- 131.** C(sp³)-H diversification of functionalized compounds [Poster Board #131]. **J. Gruhin**, E.J. Alexanian
- 132.** Using synthesis to map the human Sphingolipidome [Poster Board #132]. **C.R. Barker**, E.C. Gentry
- 133.** Stable carbon dots from microwave enabled generation of organic radicals and their additions to carbon nanoparticles [Poster Board #133]. **W. Liang**
- 134.** Novel intermolecular aziridination of unactivated olefins featuring in-situ nitrene generation under continuous flow: Preparation of N-tosyl and N-cyano aziridines as mixed amine and cyanamide precursors [Poster Board #134]. **J. Tomlin**, E. Stryker, E. Chandler, A. Chin, F. Gupton
- 135.** Nitroxyl mediated oxidation of Mycothiol [Poster Board #135]. **Y. Zeng**, S.B. King
- 136.** Toward "CO in a Pill": The effect of membrane permeability on potency [Poster Board #136]. **C. Yang**, X. Yang, W. Lu, D. Liu, R. Tripathi, B. Wang
- 137.** Incorporation and oxidative cleavage of electron rich anilines in natural peptide sequences [Poster Board #137]. **A. Watts**, C.R. Shugrue
- 138.** *Mycobacterium tuberculosis* PptT inhibitors based on heterocyclic replacements of amidinouras [Poster Board #138]. **J. Cacioppo**, S.A. Ottavi, K. Li, A. Perkowski, R. Ramesh, B. Gold, Y. Ling, J. Roberts, A. Singh, J. Zhang, J. Mosior, L. Goullieux, C. Roubert, E. Bacqué, J. Sacchetti, C.F. Nathan, J. Aube
- 139.** Can anthraquinone-based fluorophores compete with and surpass other commercially used dyes? [Poster Board #139]. **J.R. Gregory**, M.R. Korn
- 140.** Copper-catalyzed oxidative amination of alkenes using O-benzoylhydroxylamines for the synthesis of tertiary allylic amines [Poster Board #140]. **E.J. McLaren**, Q. Wang
- 141.** Assisted tandem catalytic amine synthesis using cobalt [Poster Board #141]. **T.X. Lin**, R.D. Hernandez, J.A. Tunge
- 142.** Synthesis of Thioacid functionalized photoswitchable dithienylethene derivatives [Poster Board #142]. **P. Aryal**, J. Bietsch, G. Grandhi, E. Sarabamoun, J. Choi, G. Wang
- 143.** Characteristics of fluorophores with large Stokes shifts [Poster Board #143]. **A. Sirard**, J.R. Gregory, M.R. Korn
- 144.** Facile synthesis of benzyl fluorides via Silver-catalyzed *c*-C bond fluorination of unstrained tertiary alcohols [Poster Board #144]. **I. Sprague**, M. Shah, W. Deng, V. Lindsay

- 145.** Copper-catalyzed 1,4-aminoxylation of 1,3-dienes via carbonyl-assisted oxygen migration [Poster Board #145]. **N. Watkins**, Y. Kwon, Q. Wang
- 146.** Optimization of Macmillan imidazolidinones for α -amination of aldehydes [Poster Board #146]. **C.F. Wright**, T.C. Coombs
- 147.** Target identification efforts to understand small molecule mediated unsilencing of paternal *UBE3A* [Poster Board #147]. **A. Welton-Arndt**, H. Vihma, J. Aubé, B. Philpot
- 148.** Intramolecular hydroamination and cyclization of 2,2-diphenyl-4-en-1-amine derivatives under the catalysis of Au(I)-phosphine complexes [Poster Board #148]. **R. Lan**, A.C. Jones
- 149.** Effect of coplanarity in organic semiconductors [Poster Board #149]. **J.I. Azar**, J.C. Zelenka, J.R. Gregory, M.R. Korn
- 150.** BODIPY dyes for multi-color simultaneous spectroscopic single-molecule localization microscopy [Poster Board #150]. **M. Waddington**, B. Nichols, Y. Liu, Y. Zhang
- 151.** Stereoselective aziridine ring opening with carbon nucleophiles [Poster Board #151]. **E. Brubaker**, H. Nguyen, J.B. Morgan
- 152.** Allosteric modulation of the D1 dopamine receptor as a therapeutic approach to cognitive decline [Poster Board #152]. **J. Rayadurgam**, A. Nilson, J.N. Hanson, F. Wang, D. Rogers, R.B. Free, D.R. Sibley, K.J. Frankowski
- 153.** Microwave-assisted synthesis of Wnt/b-catenin inhibitors as novel therapeutics to overcome temozolomide-resistance in glioblastoma multiforme [Poster Board #153]. **X. Weng**, N. Patel, S. Ghavami, S. Pecic
- 154.** Catalytic enantioselective synthesis of chiral xanthene analogs [Poster Board #154]. **w. tan**
- 155.** The development of Amidinuoreas, and heterocyclic analogues thereof, as *in vivo* and *in vitro* inhibitors of *Mycobacterium tuberculosis* Phosphopantethienyl transferase [Poster Board #155]. **A. Perkowski**, S.A. Ottavi, S.M. Scarry, K. Li, J. Cacioppo, R. Ramesh, J. Mosior, B. Gold, Y. Ling, J. Roberts, A. Singh, J. Zhang, L. Goullieux, C. Roubert, E. Bacqué, H. Lagiakos, J. Vendome, F. Moraca, V. Feher, J. Sacchettini, C.F. Nathan, J. Aube
- 156.** Pd nanoparticles supported on bimetallic MOFs and carbonaceous MOF-based materials for Suzuki cross-coupling reactions [Poster Board #156]. **M. Moody**
- 157.** Energy transfer catalysis for the synthesis of co-polymers [Poster Board #157]. **R. Ritter**, C. Badalis, T.A. Bender
- 158.** Amine-functionalized carbon nanotubes supported palladium nanoparticles in Buchwald-Hartwig amination [Poster Board #158]. **H.B. Winkleman**, M. Eweama, L. Picinich, **A.R. Siamaki**

159. Nickel nanoparticles supported on multi-walled carbon nanotubes; versatile catalyst for Suzuki cross-coupling reactions in batch and continuous flow [Poster Board #159]. **K.A. Coker**, H.B. Winkleman, **A.R. Siamaki**

160. Titanium catalyzed functionalization of carboxylic acids for the synthesis of chiral amines [Poster Board #160]. **S. Muhammad**, G. Gutierrez, J.A. Wilt, B. Kim

161. Harnessing proximal charges: Synthesis and application of tripodal metalloligands in homogeneous catalysis [Poster Board #161]. **A. Medley**

162. Dependence of electron transfer from Titania to Pt nanoparticles on their size and shape [Poster Board #162]. **P. Yoo**, J. Zhang, F. Polo-Garzon, Y. Sun, Z. Yang, S. Dai, H.C. Chao, M. Chi, Z. Wu, S. Irle

163. Selective palladium-catalyzed Hydroborylative intermolecular coupling of allenes enabling highly substituted 1,3-diene [Poster Board #163]. **A. Abu Anzeh**

164. Synthesis and structure of cyclopentadienes and indenenes bearing alkyl and perfluoroaromatic substituents [Poster Board #164]. **P.A. Deck**, S.A. Williams

165. Polyether catalyzed N-functionalization of amines [Poster Board #165]. **A. Storer**, A. Odoh, A. Seilkop, B. Kim

166. Elucidating the structure of pinckneyin [Poster Board #166]. **S. Varjosaari**

Durham Convention Center
Junior Ballroom A2

Analytical Chemistry Research and Development

Cosponsored by ANYL
Z. S. Davis, G. E. Potts, *Organizers*
D. Budner, I. Yawlui, *Presiding*

9:30 Opening Remarks.

9:35. Evaluation of land reclamation with MPTs at Anglogold Ashanti: A chronosequence approach. **I. Yawlui**

9:50. Geochemical fingerprinting of natural waters in Middle Tennessee. **B. Davis**

10:05. Sensing a CO-releasing molecule (corm) does not equate to sensing co. **D. Liu**, X. Yang, N. Bauer, W. Lu, B. Wang

10:20. *In vitro* isolation, characterization, and sensor development for synthetic cannabinoids. **C. Willis**, J. Canoura, Y. Liu, R. Hill, Y. Xiao

10:35 Intermission.

10:45. Magnetic field-induced modulation of the ratio of CO:H₂ in electrocatalytic CO₂ reduction. **N. Karki**, A.J. Wilson

11:00. Vapor phase diffusion of silanes: A new method to prepare stationary phase gradient on thin-layer chromatography (TLC) plate to improve chromatographic performance. **M.A. Macktuf**, M.M. Collinson, S.C. Rutan

11:15. Impact of ionic water chemistry on kombucha fermentation. **D. Budner**

11:30. In-depth study of trichloroethylene photodegradation by titanium dioxide nanoparticles: Anatase versus brookite. **V. Magyar**, O. Love

11:45. Capillary electrophoresis methods for determining binding affinities of nucleic acid enzymes in physiologically relevant buffer. **K. Irons**, D. Erie

Durham Arts Council
IBM Rehearsal Hall

Biochemistry Research and Development

Cosponsored by BIOL and BIOT

D. A. Canelas, *Organizer*

J. L. Fox, *Presiding*

9:30 Introductory Remarks.

9:35. Mechanism of the cytochrome *c* oxidase assembly factor Cox15. H.G. Addis, J.A. Carroll-Deaton, E.D. Rivett, J.V. Dietz, E.L. Hegg, O. Khalimonchuk, **J.L. Fox**

9:50. GPx4 membrane-interfacing inhibitor fragments discovered via a membrane-mimicking reverse micelle screening platform. **C.L. Labrecque**, B. Fuglestad

10:05. Synthesis and characterization of single-stranded DNA molecular recognition elements against cyanotoxin L-BMAA. **X. Santiago-Maldonado**, E. Nicolau

10:20 Intermission.

10:30. Synthesis and characterization of brucebactin-a siderophore required by *Brucella* spp. to infect pregnant cattle. **R.E. Dediavoukana**, S. Banerjee, C. Eakes, A.J. Weerasinghe

10:45. How to be a Heartbreaker: Isolating porcine heart extracellular matrix proteins by chemical and enzymatic decellularization. **L.C. Payne**, K.M. Ali, J. Gluck, T. Upadhyay, B.T. Proctor

11:00. Extending water wires to elucidate effects of pore hydration on proton channel activity. **V. Silverman**, G. Prida, H.T. Kratochvil

11:15 Intermission.

11:25. Characterization of the interaction of the regulator of G-protein signaling 10 (RGS10) and calmodulin. **K.J. Ramirez**, C. Tope Niedermaier, R. Bieber Urbauer, S. Hooks, J.L. Urbauer

11:40. Targeting membrane-mediated allosterism to develop small molecule modulators of the PLC- γ isozymes. **A.J. Carr**, Q. Zhang

Durham Convention Center
Junior Ballroom D1

Chemical Biology of Post-Translational Modifications

Cosponsored by BIOL
Y. Zheng, *Organizer*

9:30 Introduction to the symposium.

9:35. Differential regulation of SIRT5 activity by small molecules. **Y. Cen**

9:50. Discovery and characterization of PRMT1-PRMT6 interaction. **M. Cao**, Y. Zheng

10:15. Antagonist development for chromodomain-helicase DNA-binding protein 1 (CHD1). **R.L. Johnson**, A.L. Graboski, J.L. Norris-Drouin, W. Walton, M.R. Redinbo, S.V. Frye, L.I. James

10:20 Break.

10:30. Macrolactonization and macrolactamization of graspetides by ATP-grasp enzymes. **Y. Ding**

10:45. Profiling ubiquitin chain specificity by Di-ubiquitin probes. **J. Zhang**, J. Yin

11:10. Demonstration of covalent intermediates in the mechanism of peptidoglycan O-acetylation in Gram-negative bacteria. **J. London**, B. Schultz, E. Snow, S. Walker

11:15 Break.

11:25. Scalable, robust, high-throughput expression and characterization of nanobodies enabled by 2-stage dynamic control. **J. Hennigan**, R. Menacho-Melgar, M. Lynch

Durham Convention Center
Meeting Room 3

Chemistry Education Research and Practice

Cosponsored by CHED
S. L. Johnson, *Organizer, Presiding*

9:30 Introductory Remarks.

9:35. Win-win collaborative interdisciplinary course-based undergraduate research experience (ci-CURE) program for undergraduates. **G. Rabah**, S. Franzen

9:50. Microplastics as an authentic student interest research topic. **R.E. Crisp**

10:05. A REU site focusing on regional 2-yr community college students. **B. Jang**, S.D. Starnes

10:20 Break.

10:30. Teaching protein structure and function using the basil biochemistry cure. **J.D. Dattelbaum**

10:45. Design, synthesis, and analysis of a peptide specific for the “WU1896” receptor: An undergraduate biological chemistry laboratory experiment to teach rational drug design and solid phase peptide synthesis. **K.R. Wilson**

11:00. Design and assessment of virtual interactive cell culture laboratory training experiences for accessible Biotechnology. E. Cartwright, D. Spencer, C. McGowen, D. Tredwell, C. Potts, N. Sudduth, E. Brown, P. Albright, A. Jhala, **M.C. Srougi**

11:15 Break.

11:25. Chirality explored in the sophomore organic chemistry laboratory. **M.R. Korn**

11:40. A reflection on integrating artistic and communicative topics with common physical chemistry misconceptions. **M. Lam**, J. Donnelly

11:55. CERISE: Chemical education realized through interactive storytelling experiences. A. Rhodes, C. Solomon, **D.C. Ashley**

Durham Convention Center
Junior Ballroom A3

Computational Chemistry: Educational Impact and Research Advances

Cosponsored by CHED

D. A. Canelas, S. C. Sendlinger, *Organizers*

R. R. Gotwals, R. M. Whitnell, *Presiding*

9:30 Introductory Remarks.

9:35. Computational chemistry education: Beakers aren't enough. **R.R. Gotwals**

9:50. Using DFT calculations in the physical chemistry laboratory. **T.C. Devore**

10:05. A small program to extend the conjugated dyes experiment. **A. Mansell**

10:20 Break.

10:30. Guided inquiry computational chemistry experiments for the physical chemistry lab from the POGIL-PCL project. H.L. Berghout, A. Grushow, S.S. Hunnicutt, M.J. Perri, M.S. Reeves, **R.M. Whitnell**

10:45. Classifying asphaltenes with machine learning as a CURE module. **A.K. Sharma**

11:00. Quantitative evaluation of halogen bonding in d-block halides: A computational analysis. **N.H. Pham**, K. Donald

11:15. Electrocatalytic Reduction of CO₂ to CH₄ using X₂DEBDC (X = Fe, Mn; E = O, S) materials: A comprehensive computational investigation. **G. McCarver**, T. Yildirim, W. Zhou

Durham Arts Council
PSI Theatre

Inorganic Chemistry Research and Development

Cosponsored by INOR

J. M. Harrington, *Organizer*

9:30 Opening Remarks.

9:35. Alkoxide-Phosphine supported Early-Late heterobimetallic Complexes. **S. Vijayan**

9:50. Main group element-based dithiolene complexes: From radicals to zwitterions. **P.M. Tran,** Y. Wang, G.H. Robinson

10:05. ORR activity of diluted doped Zinc oxide materials with first row transition metals. N.M. García-Rodríguez, C. Quiñones-Martínez, H. González-Vélez, J.J. Soto-Ortiz, H.D. Abruna, **M.B. Santiago-Berrios**

10:20 Break.

10:30. Mechanism of interfacial proton-coupled electron transfer for metal-aquo bond formation with applications in artificial photosynthesis. **M. Kessinger,** J. Xu, Q. Loague, J.T. Sirlin, G.J. Meyer

10:45. Preparation of novel chalcogenide materials: Single-crystal-to-single-crystal post-synthetic modification. **A. Berseneva,** H. zur Loye

11:00. The role of anisotropy and crystal structure on the behavior of magnetic core@shell nanoparticles. **D. Carnevale**

11:15 Break.

11:25. Electronic structure and excited state reactivity of d^5 metallocene complexes with LMCT excited states. **A. May,** G.M. Curtin, M. Deegbey, E. Danilov, F.N. Castellano, E. Jakubikova, J.L. Dempsey

11:40. A diiron imido complex capable of C–H Bond activation. **R. Gwinn,** D. Thornton

11:55. Synthesis, characterization, and reactivity of Bis(alkoxide) iron complexes. **M. Williams,** R. Gwinn, D. Thornton

12:10. Tetrameric Ln_2Fe_2 complexes ($Ln = La, Pr, Gd, Ho, Tb$) as models of coupled molecular spin qubits. **S. Bisht,** W. Chou, S. Hill, M. Shatruk

12:25. Development of light-activated inhibitors and Ru-PROTACs for cytochrome P450. **D. Havrylyuk,** D.K. Heidary, P.C. Glazer

Durham Convention Center
Junior Ballroom A1

New Chemistries for Redox Flow Batteries

Cosponsored by INOR
C. Bejger, *Organizer, Presiding*

9:30 Opening Remarks.

9:35. Advanced nanostructured cathodes for high energy density and long-life lithium-sulfur batteries. **M. Kaid**, H.M. El-Kaderi

9:55. Fungal secondary metabolites for organic redox flow batteries. **S. Hematian**, M. Tapia, R. AL-QIAM, N.H. Oberlies

10:15. Radical dimerization in [3]radialene aqueous catholytes. **C. Bejger**, F. Hasan

10:35 Break.

10:40. Leverging ligand-coupled electron transfer for the development of two-electron inorganic catholytes for redox-flow batteries. **B.H. Farnum**

11:00. Membrane-free redox flow batteries. **J. Jiang**

Durham Convention Center
Junior Ballroom C

Organic Chemistry Research and Development

Cosponsored by ORGN
D. A. Canelas, K. C. Glasgow, *Organizers*
C. Saint-Louis, *Presiding*

9:30 Opening Remarks.

9:35. Solvatochromic and aggregation-induced emission (AIE)-active Nitro phenyl-substituted pyrrolidinone-fused 1,2-azaborine conjugates: A molecular design strategy. **C. Saint-Louis**

9:50. Boronic acid catalysts for the hydroboration of alkenes. **S. Mummadi**, C. Richardson, D. Rose, C. Krempner

10:05. Efficient and selective synthesis gem-difluoro substituted arenes by Defluoroallylation with boron-stabilized nucleophiles. **J.L. Rosario**, S. Meek

10:20. Balancing reactivity, regioselectivity, and product stability in Ir-catalyzed ortho C–H borylations of anilines by modulating the diboron partner. J.R. Montero, **A. Yadav**, S. Lee, B. Ghaffari, M.R. Smith, R.E. Maleczka

10:35 Break.

10:45. Application of alkynyl-Prins reactions: Atom-economical cascade sequence to fused, tetracyclic dihydrochromeno[3,4-c]chromenes. **R.J. Hinkle**, K. McFadden, C.L. Burns, K.U. Kim

11:00. Design, synthesis and biological evaluation of natural product-based hybrids. **A. Pham**, B.L. Lokeshwar, S.S. Panda

11:15. Michael Reaction to generate enantioenriched heterocycles. **J. Carsley**

11:30 Break.

11:40. Styrene synthesis via crossed aldehyde-aldehyde aldol coupling promoted by trimethylsilyl trifluoromethanesulfonate. **C.W. Downey**

11:55. Highly efficient and recyclable nickel nanoparticles supported on multi-walled carbon nanotubes for Suzuki cross-coupling reactions in continuous flow. **A.R. Siamaki**, K.A. Coker, H.B. Winkleman

12:10. Mechanistic manifold in a hemoprotein-catalyzed cyclopropanation reaction with diazoketone. R.L. Khade, **Y. Zhang**

12:25. Direct synthesis of dimethyl carbonate from CO₂ and methanol using CeO₂-ionic liquid modified catalyst. **B.B. Asare Bediako**, **N. Labbé**, **N. Abdoulmoumine**, M. Li

Durham Convention Center
Junior Ballroom D2

Polymer Chemistry and Materials Science Research and Development

Cosponsored by PMSE and POLY
D. A. Canelas, *Organizer*
J. Budhathoki-Uprety, *Presiding*

9:30 Introductory Remarks.

9:35. Developing polymers to reduce water pollution from synthetic dyes. **J. Budhathoki-Uprety**, M. Lord

9:50. Synthesizing modular hyperbranched glycomaterials with terminal sialic acid or mannose moieties for inhibiting influenza infections. **J. Mase**, R. Bianculli, J. Rubino, M.D. Schulz

10:05. Expanding the library of peptidic dendrimers via accelerated synthetic methods. **J. O'Brien**, C.B. Gorman, S. Menegatti

10:20 Break.

10:30. Modifying PAMAM dendrimers for drug delivery. **D. Leonard**, C.B. Gorman

10:45. Comparison of initiators towards the synthesis of degradable Poly(styrene-co-acetal) from bio-based precursor. **a.m. valencia**, C.N. Scott

11:00. RAFT step-growth polymerization and RAFT interchange. **J. Tanaka**, W. You, J. Li, S. Clouthier

11:15 Break.

11:25. Design and synthesis of triphenylphosphine containing macromolecular catalysts for determination of structure-function relationships. **M. Sanders**, S. Chittari, N. Sherman, J. Foley, A. Knight

11:40. Fully organic, radioluminescent nanoparticles with emission spanning the full visible spectrum and into the near-infrared via x-ray induced, sequential Förster resonance energy transfer: Color manipulation via a photonic bandgap and bioimaging applications. **H.W. Jones**, I. Bandera, I.K. Foulger, S.H. Foulger

11:55. Polyaddition of maleimides and Maleiamides via hydroamination. N.Z. Singleton, E.R. Anderson, M.M. Spandau, **H.J. Schanz**

Durham Arts Council
Adaron Hall

Ultrafast and Nonlinear Spectroscopy

Financially supported by Light Conversion, Ultrafast Systems, and Phase Tech Spectroscopy

T. Lian, L. Wang, *Organizers*

E. Ghadiri, *Presiding*

9:30 Introductory Remarks.

9:35. Pump-probe microscopy provides novel contrast for melanoma diagnosis. **W.S. Warren**

9:55. Vibrational probe of mobility of hydrophobic region of lipid bilayers at specific depth. **I.V. Rubtsov**, M. Islam, S. Nawagamuwage

10:15. Two-dimensional, ultrafast kinetics: Micelle dynamics and structure. M. Dhar, B. Manna, **M.A. Berg**

10:35 Intermission.

10:45. Effects of proaromaticity on excited-state properties in near-infrared sensitizer dyes. **N. Hammer**, N. Kruse, A.L. Dorris, J.H. Delcamp, G.S. Tschumper

11:05. Time-resolved optical probe and control of coherent states in multifunctional materials at high magnetic fields. **G. Khodaparast**

11:25. The effect of sulfur substitution on the photoprotective properties of pyrimidine nucleobases. **S. Ullrich**, A. Mohamadzade, Y. Qu

Durham Convention Center
Junior Ballroom D3

Green Chemistry-Driven Fundamental Research & Development of Nanocelluloses

Cosponsored by CELL
L. A. Lucia, L. Pal, *Organizers*

9:45 Introductory Remarks.

9:50. Advances in integrated biorefinery systems for waste valorization. M. Salas, N. Haque, R. Rao, A. Mittal, J. Yarbrough, L.A. Lucia, **L. Pal**

10:05. Analysis of the synthetic method and adsorptive properties of a sustainable cellulose nanomaterial. **C. Kwiatkowski**, E. Hayden, J.C. Poler

10:20. Cellulose nanofibrils stabilized water-in-oil Pickering emulsions for encapsulation of phytic acid and inorganic salt hydrate. **S. Mubarak** , Y. Kim

10:35 Intermission.

10:45. Modified cellulose nanocrystals used for metal ion removal to refine biodeisels. **R. Marasco**, G. Gardner, E. Vidal, C.D. Garcia, D.C. Whitehead

11:00. Manipulation of ionic liquid solvent -biopolymer interactions for the regeneration of biocompatible materials. **E. McDowell**, L.D. Yoder, J. Brown, K. Dellinger, J.R. Alston

11:15. Improving biopolymer dissolution in ionic liquids for biomedical applications. **L. Yoder**, E. McDowell, J. Knoop, B. Sadiku, J.R. Alston

11:30. Standardization of the viscosity and cellulose concentration relationship for reproducible cellulose in 1-butyl-3-methylimidazolium chloride solutions. **J. Coscarelly**, E. McDowell, L.D. Yoder, J.R. Alston

11:45 Closing Remarks.

Durham Convention Center
Meeting Room 4

Coordination Chemistry, Synthesis, Characterization and Reactions

Cosponsored by CATL, INOR and ORGN
Financially supported by Coastal Georgia Local Section
W. E. Lynch, *Organizer*

10:00 Opening Remarks.

10:05. Iron complexes with tridentate ligands for coordination chemistry, bioinorganic and catalytic studies. **W.E. Lynch**, G. Roberts, C.W. Padgett, B.P. Quillian

10:25. Silver coordination chemistry: Synthesis and structures of new N-heterocyclic thione and selone complexes. **D. Rabinovich**

10:45. Incorporating second-sphere hydrogen bonding in metal-sulfonamidate complexes for capture of hydrogen sulfide. **C.M. Wallen**

11:05 Intermission.

11:15. Preparation, characterization, reactivity and coordination properties of N,N'-(1,2-phenylene)*bis*(pyrazol-1-yl)acetamide ligands derivatives. **B.P. Quillian**, E.C. Abbott, P.H. Ouedraogo, A. Bryant

11:35. In support of N-O transition metal chemistry: Utilizing the *N*-oxide functional group to tune the properties of coordination complexes. **J.A. Pienkos**, C. McMillen

Durham Convention Center
Grand Ballroom I

Analytical Chemistry Research and Development Poster Session

Cosponsored by ANYL
Z. S. Davis, G. E. Potts, *Organizers*

11:10 - 1:10

- 101.** Qualitative detection of illicit drug use in hair samples via GC/MS [Poster Board #101]. **P. Griffeth**, C.H. Lisse
- 102.** Evaluation of cyclic voltammetry measurements of antiarrhythmic drugs [Poster Board #102]. **L. De La Garza**, D.N. Thomas
- 103.** Effects of cigarette smoke in the lungs: Its major role in defective mitophagy and premature senescence [Poster Board #103]. **M.J. Santiago**, M. Imran, Z. Grand, S. Chinnapaiyan, M.S. Rahman, K. Panda, H.J. Unwalla
- 104.** Adsorptive removal of organophosphate pesticides using carbon nanofibers obtained from electrospinning [Poster Board #104]. **B. Adesanmi**, S.O. Obare, J. Wei
- 105.** Redox-activated prochelators with antifungal activity against *Candida albicans* under fluconazole stress [Poster Board #105]. **M. Merriman**, Y. Sung, E. Tomat, K.J. Franz
- 106.** Molecularly imprinted polymers as sensitive nanosensors for organophosphate pesticide detection [Poster Board #106]. **R.D. Ayivi**, J. Wei, S.O. Obare
- 107.** Amplification-by-polymerization in VOC sensing [Poster Board #107]. **D. McCoy**, P. He
- 108.** Comparison of analytical techniques in analysis of human breast milk composition [Poster Board #108]. **E. Thornton**, B. Hardy, R. Claro Da Silva, K. Subedi, H. Colleran
- 109.** Engineering a SERS enabled microfluidics biosensor for the analysis of EVs derived proteins [Poster Board #109]. **S. Al Abdullah**, M. Raza, R. Zadegan, K. Dellinger
- 110.** Investigating cellular and tissue transport properties of target-activated fluorescent probes for assisting fluorescence guided surgery [Poster Board #110]. **S. Mukherjee**, S. Jomy, R.L. McCarley
- 111.** Advancing fluorescence imaging for cancer diagnosis and treatment: Near-infrared fluorescent probe for accurate visualization of cancer cells via Hnqo1 responsiveness [Poster Board #111]. **S. Jomy**, S. Mukherjee, R.L. McCarley
- 112.** Effect of Trans-3,5,4' - trihydroxystilbene (resveratrol) on oxidative stability of extra virgin olive oil under accelerated aging conditions [Poster Board #112]. **A. Anderson**
- 113.** Difluoroacetamide: A selectively-tunable, universal ^1H and ^{19}F quantitative NMR standard [Poster Board #113]. **J.S. Wood**, R. Cohen, X. Wang, M. Reibarkh, R.T. Williamson
- 114.** Solution-cathode glow discharge as a source of molecular and atomic emission [Poster Board #114]. **N.M. Radomski**, D.S. Vaidya, M.R. Webb

115. Gold nanopattern array as a rigorous reference standard for calibrating spectroscopic single-molecule localization microscopy and aberation correction [Poster Board #115]. **M. Shahid**, Y. Liu, Y. Zhang

116. Cellulase immobilized to magnetic nanoparticles: Comparison of adsorption and covalent attachment [Poster Board #116]. **T. Le-Vasicek**, G. Coulter, S. Fink, C. Snavely

117. Multiplexed surface protein detection and cancer classification using gap-enhanced magnetic-plasmonic core-shell Raman nanotags [Poster Board #117]. **A. Rodriguez-Nieves**, M.L. Taylor

118. Analysis of iron and chromium in organic and inorganic cumin and coriander powders using atomic absorption spectrometry (AAS) [Poster Board #118]. **M. Subramaniam**

119. Rapid method for the rapid detection and quantification of steroidal lactones in Ashwagandha [Poster Board #119]. V. Lescano, D.J. Rumley, **T.T. Griffin**

120. Local electrochemical probing along with surface topography of the targeted nanoparticles in air via combined SECCM and AFM under visual monitoring [Poster Board #120]. **M. Ashaduzzaman**, S. Pan

121. Thermal-desorption electrospray-mass spectrometry (TD-ESI-MS) for dye analysis [Poster Board #121]. **J. Wu**, X. Sui, B. Musselman, N.R. Vinueza

122. Comparison of aptamer binding properties determined by exonuclease digestion and strand-displacement assays [Poster Board #122]. **A. Bryant**, Y. Xiao

123. Characterizing *Artemisia annua* by IR-MALDESI utilizing three different optical trains [Poster Board #123]. **S. Ashbacher**, Q. Mills, A. Sohn, D.C. Muddiman

124. Direct analysis of wastewater from dyeing processes by paper spray mass spectrometry [Poster Board #124]. **A. Trettin**, N.R. Vinueza

125. Optimizing tissue preparation for IR-MALDESI mass spectrometry imaging (MSI) of neurotransmitters [Poster Board #125]. **M. Wang**, Y. Ouyang, T. Segura, D. Muddiman

126. Atomic emission (AES) analysis of gunshot residue (GSR) as a function of distance and target background [Poster Board #126]. **S.E. Hooper Marosek**, V. Antharam, D. Pauly, A. Wilcox

127. Chitosan carbon dots for selective binding and sensing of PFAS [Poster Board #127]. **X. Huang**, C.L. Colyer

128. Detection of synthetic musk compounds in indoor dust by in-tube extraction dynamic headspace (ITEX-DHS-GC-MS) [Poster Board #128]. **O. Ifedayo**, A.F. Callender, B. Olope

- 129.** Exploratory analysis of organic pollutant in household dust by Mae-GC/MS/MS [Poster Board #129]. **B. Olope**, A.F. Callender, O. Ifedayo
- 130.** Efficient energy harvesting in N719 dye and Ni-MoSe₂/2D nanomaterials-based dye-sensitized solar cells [Poster Board #130]. **M.H. Kabir**, A. Steadman, M. Shohag
- 131.** Simple method for determining the authenticity of Saffron by ultraviolet/visible spectroscopy [Poster Board #131]. **V. Pham**, J. Peterson, R. Fell, K.W. Barnes
- 132.** Analysis of pre-workout [Poster Board #132]. **I. Ramirez**, K.W. Barnes
- 133.** Effect of brookite TiO₂ nanoparticles size on photocatalytic degradation of perfluorooctanoic acid (PFOA) [Poster Board #133]. **L. Dippy, O. Love**
- 134.** Characterization of food supplements using mid-infrared spectrometry, Folin-Ciocalteu reagent, and direct real time mass spectrometry [Poster Board #134]. **M. Dodson**, H.Z. Msimanga, P. Owusu, L. Reynolds, S. Mincey
- 135.** Electrocatalytic reduction of hydrogen peroxide at paraffin-sealed nitrogen-doped carbon fiber ultramicroelectrodes [Poster Board #135]. **Y.G. Mohammed**
- 136.** Electrochemiluminescence using pencil graphite electrodes and screen-printed carbon electrodes interfaced with a simple imaging system [Poster Board #136]. **S.O. Ehigiator**, G.W. Bishop
- 137.** Quantification of cholesterol esters during mouse brain development [Poster Board #137]. **A. Elliott**, D. Dedunupitiya, E. Go, H. Kobayashi, M.D. Hartley
- 138.** Implantable electrochemical sensor for sensitive and selective nitric oxide detection in vivo [Poster Board #138]. **M. Nogler**, M. Schoenfish
- 139.** Formation and dynamic evolution and stability imaging of solid electrolyte interface (SEI) of lithium-ion batteries (LIBs) with scanning electrochemical microscopy [Poster Board #139]. **E. Wornyo**, S. Pan
- 140.** Developing a CE-LIF method for the determination of norepinephrine levels in the brain's locus coeruleus, in a study of decreased cognitive function and mobility with aging [Poster Board #140]. **K. Morgan**, E. Budygin, O. Delbono, C.L. Colyer
- 141.** Electrochemical CO₂ reduction at surface modified silver nanoparticles [Poster Board #141]. **I. Trevino**, S. Pan
- 142.** Fabrication of an instrumented fetal membrane on-a-chip (Ifmoc) and the electrochemical analysis of the fetal-maternal interface [Poster Board #142]. **H. Richards**, J. Martin, O. Owens, G. Buckey, D.E. Cliffl

143. Investigation of the optical properties of dye molecules for aptamer-based dye-displacement assays [Poster Board #143]. **A. Sweilam**, R. Hill, T. Nguyen, Y. Xiao

144. Quartz crystal microbalance analysis of microplastic solutions [Poster Board #144]. **S. Lynch**, C. McCloy, M. Curtis, E. Stewart, J. Burgess

145. An investigation of the generality of an aptamer-based MTC displacement assay [Poster Board #145]. **M. Venzke**, A. Bacon, Y. Xiao

146. Comprehensive study of the generality of aptamer-based dye-displacement assays [Poster Board #146]. **P. Ly**, Z. Millbern, N.R. Vinueza, Y. Xiao

147. Sensitive cocaine detection utilizing aptamer-dye complexes [Poster Board #147]. **T. Nguyen**, Y. Xiao

148. Development and validation of analytical methods to quantitate PFAS compounds in gavage dose formulations for rodent toxicology studies [Poster Board #148]. **T. Bui**, J.C. Blake, **D. Coleman**, J. Ambroso, L. Adams, J. Tomayko

149. Method assessment for the determination of methoxy content in methycellulose used in aqueous dosing vehicles [Poster Board #149]. **J. Fouse**, J.C. Blake, **J. Licause**, R.A. Fernando, M. Silinski

150. Analytical research & development at Merck: Leveraging diverse expertise to be partners in problem solving [Poster Board #150]. **K. Feibelman**

151. Development of core-shell nanoparticles for surface-enhanced Raman spectroscopy (SERS)-based bio-assays [Poster Board #151]. **F.M. Lenahan**, K. Ledford, A. Wood, B. Sharma

152. Evaluation of deep eutectic solvents (DES) as green extraction materials to remove polycyclic aromatic hydrocarbons (PAHS) [Poster Board #152]. **K. Jorgensen**, R.L. Pérez

153. Determination of toxic heavy metals in coffee samples [Poster Board #153]. M. Simmons, **S. Melaku**

154. Wears Valley wetland's impact on water quality [Poster Board #154]. **M. Walker**, D. Unger, N. Duncan

155. Characterization of commercial *Cannabis sativa* L. products for authenticity using untargeted metabolomics [Poster Board #155]. **F. Rotich**, P. Manwill, N.B. Cech

156. Optimization and safety assessment of bench-scale borazine synthesis [Poster Board #156]. **A. Contreras**, V. Arredondo, A.R. Hopkins, J.R. Alston

THURSDAY AFTERNOON

Durham Arts Council
Duke Rehearsal Hall

Innovative Ways to Communicate the Value of Chemistry to The Public

Cosponsored by CPT

Financially supported by CPRC: Committee on Public Relations and Communications

S. R. Goode, *Organizer, Presiding*

9:30 Introductory remarks.

9:35. Chemistry outreach 2-102!. **A.A. Hazari**

9:55. Communication resources of the American Chemical Society. **S.R. Goode**

10:15 Intermission.

10:25. Science outreach program at the University of Tennessee Southern. **T. Cosby, E. Badolato**

10:45. Harnessing the power of data: Unleashing the potential of the US EPA Comptox Chemicals Dashboard through public APIs. A. Rashid, **A.J. Williams**

11:05 Panel Discussion.

Durham Convention Center
Junior Ballroom A2

Analytical Chemistry Research and Development

Z. S. Davis, G. E. Potts, *Organizers*

M. Limbach, *Presiding*

1:00 Introductory Remarks.

1:05. Developing a robust methodology for structural elucidation: Uncovering physical and chemical properties of cyclosporines. **M. Limbach**, E. Lindberg, H. Olivos, C. Steren, T. Do

1:20. Halogen bonding based molecular detection with functionalized gold nanoparticles – analytical sensors for environmental and forensic targets. M.M. Sherard, J.S. Kaplan, K. Lalwani, Q. Dang, S. Reiff, J. Simpson, **M.C. Leopold**

1:35. Nuclear forensic analysis of Manhattan Project plutonium. **C.M. Folden**

1:50 Intermission.

2:00. High surface area rice husk biochar for supercapacitor electrodes. **J.M. Hewage**, P.M. Rodrigo, T.E. Mlsna, D. Wipf

2:15. Fluorescence probe spectroscopy for in situ characterization of submicron particles. **P.E. Ohno**

Durham Arts Council
IBM Rehearsal Hall

Biochemistry Research and Development

Cosponsored by BIOL and BIOT

D. A. Canelas, *Organizer*

E. Brunk, *Presiding*

1:00 Introductory Remarks.

1:05. Towards a functional understanding of extrachromosomal DNA (ecDNA). **E.C. Brunk**, J. Chen, Y. Wang, C. Ford, O. Cope

1:20. Modulation of doxorubicin-induced nephrotoxicity by olmesartan and/or L-carnitine. **M. Aziz**, M. Abd El Fattah, H. Sayed

1:35. Sequential mixing stopped flow method to investigate the kinetic mechanisms of protein translocation catalyzed by ClpB. **J. Banwait**, A.L. Lucius

1:50. Chemical modifications of nucleic acid nanoparticles modulate immunostimulatory properties. **J. Hardrick**, Y. Avila , M. Panigaj, K. Afonin

2:05 Break.

2:15. Folic acid coated solid lipid nanoparticle drug encapsulation of paclitaxel: A study of particle size consistency and drug loading capacity. **L. Richmond**

2:30. Structural hindsight of lipid chaperone proteins using mimicking membrane models. **a. castillo**, G. Zorn, B. Fuglestad

2:45. Programmable microfluidic-based synthetic bacterial communities. **S. Oliveira**

3:00. Effect of nitroxyl (HNO) on *Bacillus subtilis* redox homeostasis. **Z. Xia**, P.C. Dos Santos, S.B. King

Durham Convention Center
Junior Ballroom A3

Data Analysis Workflows for Non-Targeted Analysis Studies

Cosponsored by CCPA
A. Chao, A. Williams, *Organizers*

1:00 Introductory Remarks.

1:05. Developing an EPA database of open spectra to support non-targeted analysis. **G. Janesch**, E. Carr, V. Samano, B. Meyer, L. Roach, J.P. McCord, A. Chao, T. Ferland, J. Sobus, A. Williams

1:20. Non-targeted analysis of extractable and leachable additives from microplastics prepared from reference polymer materials. **A. Lewis**, J. Sipe, M. Wiesner, L. Ferguson

1:35. EPA's non-targeted analysis webapp: Aligning web-based software tools with best practices for NTA. **A. Chao**, J.M. Minucci, M. Boyce, T. Cathey, S.T. Purucker, T. Ferland, E.T. Carr, G. Janesch, A. Williams, J. Sobus

1:50 Break.

2:00. Suspect screening analyses of silicone wristbands highlight gender disparities in chemical exposures. **N. Herkert**, J. Levasseur, K. Hoffman, G.J. Getzinger, L. Ferguson, A. Young, J.G. Allen, H.M. Stapleton

2:15. Annotating and visualizing a database of analytical methods. **E.T. Carr**, G. Janesch, S. Sivasupramaniam, J.P. McCord, L. Roach, A. Chao, J. Sobus, A. Williams

2:30. Quality assurance and quality control workflow for the non-targeted analysis of de facto water reuse. **N. Sayresmith**, L.D. Brunelle, A.L. Batt, A. Chao, E.T. Carr, T. Cathey, J.P. McCord, J.M. Minucci, S.T. Purucker, A. Rashid, D. Smith, A. Williams, D.A. Alvarez, E.T. Furlong, S.T. Glassmeyer, D.W. Kolpin, M.A. Mills, J. Sobus

2:45. Cheminformatics tools and chemistry data underpinning mass spectrometry analyses at the US Environmental Protection Agency. **A.J. Williams**, G. Janesch, E.T. Carr, C. Lowe, N. Charest, T. Martin, V. Tkachenko, A. Chao, J.M. Minucci, A. Rashid, J. Sobus

Durham Convention Center
Junior Ballroom A1

DEIR Lightning Strides in the Chemical Enterprise

Cosponsored by CMA

A. Lopes, T. Williams, *Organizers*

1:00 Introductory Remarks.

1:05. Intersecting identities and the stem environment: An examination of how diverse groups of low-income students navigate collegiate stem environments. **R.D. Davis**, Z.S. Wilson-Kennedy

1:25. The LS-PAC models center: Addressing the critical need for diversity in STEM academia through structured mentoring networks. **K. Williams, W. Johnson**

1:45. Bright IDEAS: How to cultivate and sustain a diverse and inclusive STEM workforce. **J. Pritchett**

2:05 Break.

2:15. Using employee resource groups to conquer the eighteen inch gap. **C. Ribes**

2:45. Reimagining environments that support BIPOC students' elevation: Developing a mentoring network for broader participation. **T. Williams**

Durham Arts Council

Duke Rehearsal Hall

Single-molecule Dynamics in Complex Chemical and Biological Systems

Cosponsored by ANYL, BIOL, BIOT and PHYS

A. Gahlmann, K. Welsher, *Organizers*

1:00 Introductory Remarks.

1:05. Placing molecules in context with correlative single molecule imaging and lattice light sheet microscopy. T. Daugird, Y. Shi, **W. Legant**

1:25. High-speed 3D tracking and imaging microscopy captures early events of the virus-cell interaction. **C." Johnson**

1:45. Hour-long, kilohertz sampling rate 3D single-virus tracking in live cells via StayGold fluorescent protein labelling. **Y. Lin**, J. Exell, H. Lin, C. Zhang, K. Welsher

2:00 Break.

2:10. Single-molecule fluorescence spectral heterogeneity: The probe or the environment?. **Y. Zhang**

2:30. Blink-based multiplexing: Rapid classification of spectrally-overlapped single emitters using their blinking. **K.L. Wustholz**, A. Khodabocus, A.G. Seabury, E. Smith, G.R. Hoy, G. DeSalvo

2:45. Distinct complexes containing the cytosolic type III secretion system ATPase SCTN resolved by 3D single-molecule tracking in live *yersinia enterocolitica*. **O.I. de Cuba**, J.R. Prindle, C.F. Tyndall, A. Gahlmann

3:00. Single-molecule tracking to determine the abundances and stoichiometries of freely-diffusing protein complexes in living cells. **J.R. Prindle**, O.I. de Cuba, A. Gahlmann

Durham Convention Center
Junior Ballroom B

Southeastern Magnetic Resonance Conference (SEMRC)

Cosponsored by ANYL and PHYS
A. I. Smirnov, M. A. Ter Horst, *Organizers*

1:00 Introductory Remarks.

1:05. Elucidating chemistry and biology of site-specific DNA damage by NMR. **M.P. Stone**, Y. Fu, R. Tomar

1:20. Irregular secondary structures in small peptides. **M.W. Giuliano**

1:35. Defining key interactions between host cell immunophilins and SARS-CoV-2 nsp1. M.E. Blake, L. Clark, P.E. Prevelige, **C.M. Petit**

1:50. Noninvasive early detection and stage of chronic lung diseases with precision MRI (pMRI). **D. Li**, O.Y. Ibhagui, h. han, G. Peng, M. Meister, Z. Gui, J. Qiao, S.o. Bamishaye, F. Akinlotan, Y. Yuan, H. Yang, S. Tan, S. Xue, K. Hekmatyar, H. Grossniklaus, P. Sun, Y. Meng, X. Ji, Z. Liu, J. Yang

2:05 Break.

2:15. Continuous arterial spin labelling in vivo imaging at 21.1-T. **K. Birch**, M. Elumalai, S. Grant, D. Ritcher

2:30. Non-invasive mapping of molecular determinants for liver cancer and metastatic aggressiveness by precision MRI (PMRI). **Z. Gui**, J. Qiao, S. Tan, H. Yang, F. Mishra, L. Tian, D. Li, Y. Meng, N. Wang, K. Hekmatyar, Y. Xie, P. Sun, E. Seki, Z. Liu, D. Li, H. Grossniklaus, J. Yang

2:45. ACERT: A service resource for ESR researchers. **M. Srivastava**

3:00. High-spin manganese(III) coordination complex serving as a useful tool in terahertz / ultra-high field EPR. t. dubroca, S. Hill, J.A. Telser, **J. Krzystek**

Durham Arts Council
PSI Theatre

Inorganic Chemistry Research and Development

Cosponsored by INOR
D. A. Canelas, K. C. Glasgow, J. M. Harrington, *Organizers*

1:15 Introductory Remarks.

1:20. Methyl-termination suppresses competitive hydrogen evolution reaction at p-Si photoelectrodes for photoelectrochemical CO₂ reduction by a molecular ruthenium catalyst. **G.P. Bein**, M. Stewart, E.A. Assaf, S.J. Tereniak, S. Fernandez, R.N. Sampaio, A.J. Miller, J.L. Dempsey

1:35. High-pressure synthesis of Nd₂Re₄Bo₈ for nuclear waste studies. **Z. Hussein**, N. Kazemiasl, K. Hussaini, L. Vaquero, O. Ibragimova, S. Chariton, V. Prakapenka, I. Chuvashova

1:50. Cyanogel templating method for the synthesis of PD-CR bimetallic electrocatalyst for CO₂ reduction. **T.O. Salami**, K.M. Icard

2:05. Nanosecond intra-ionic chloride photo-oxidation. A. Deetz, **M. Goodwin**, E.A. Kober, G.J. Meyer

2:20 Intermission.

2:30. Catalytic CO₂ reduction using Cu-coordinated, crystalline carbon nitride. **M. Pauly**, M. Deegbey, L. Keller, S. McGuigan, G. Dianat, J. Wong, C. Murphey, B. Shang, H. Wang, J. Cahoon, R.N. Sampaio, Y. Kanai, G. Parsons, E. Jakubikova, P.A. Maggard

2:45. Lewis acid-formyl adducts with enhanced durability and reactivity. **J.T. Sirlin**, A. Muller, A. Deetz, N. Kumarage, M.Z. Ertem, G.J. Meyer, J.J. Concepcion, R.N. Sampaio

3:00. Synthesis and characterization of molybdenum(III) amidinate for aerosol-assisted chemical vapor deposition (AACVD) and atomic layer deposition (ALD) applications. **T.M. Currie**, Z. Ali, L. McElwee-White, T. Jurca

Durham Convention Center
Junior Ballroom C

Organic Chemistry Research and Development

Cosponsored by ORGN
D. A. Canelas, *Organizer*
M. Bonizzoni, J. M. Bray, *Presiding*

1:15 Opening Remarks.

1:20. Phenolic acids as binding probes for cyclodextrin complexation. X. Yao, **M. Bonizzoni**

1:35. Synthetic strategies towards Chevalinulins A and B. **J.M. Bray**, G. Adornato, K.M. Lambert

1:50. Diversification of biomolecules via SuFEx activation of embedded hydroxy motifs. **A. Odoh**, B. Kim

2:05. Synthesis and characterization of novel meridional naphthyridine-derived ligands. **A. Hernandez**, J. Stober, D.P. Harrison

2:20 Break.

2:30. Ru-catalyzed enantioselective synthesis of chiral xanthene and relevant structure. **w. tan**

2:45. Asymmetric deoxygenative functionalization of carboxylic acids via titanium-multicatalysis. **G. Gutierrez**, J.A. Wilt, B. Kim

3:00. Site- and diastereoselective synthesis of homoallylic alcohols containing quaternary carbon centers by nickel-catalyzed dicarbofunctionalization. **B. Swartz**, S. Meek

Durham Convention Center
Junior Ballroom D2

Polymer/Polymerization-Based Biosensing and/or Bioimaging Techniques

Cosponsored by PMSE and POLY
P. He, K. Johnson, *Organizers, Presiding*

1:15 Introductory.

1:20. Polymer use in biomedical imaging: Imaging Physics. **K. Johnson**

1:40. Ultrasensitive biosensing and tumor bioimaging via bio-responsive self-assembling supramolecules and multifunctional nanointerface. **X. Wang**

2:00. Sequence derived control over structure and function of di(phenylalanine) polymer nanoparticles. **P. Dykeman-Bermingham**, M. Bogen, S.F. Grizzard, A. Knight

2:20. Amplification-by-polymerization in DNA biosensing. **P. He**

Durham Arts Council
Adaron Hall

Ultrafast and Nonlinear Spectroscopy

Cosponsored by ANYL
Financially supported by Light Conversion, Ultrafast Systems, and Phase Tech Spectroscopy
E. Ghadiri, T. Lian, *Organizers*
L. Wang, *Presiding*

1:15 Introductory Remarks.

1:20. Advanced ultrafast optical spectroscopy and microscopy for photochemical analysis of complex energy conversion materials and devices. **E. Ghadiri**

1:40. Ultrafast dynamics of Cu(I)-based earth-abundant photosensitizers. M.C. Rosko, N. Durand, J.P. Wheeler, R.T. Alameh, A.P. Faulkner, S. Kromer, **F.N. Castellano**

2:00 Intermission.

2:10. Ultrafast spectroscopy on metal-organic framework confined molecular chromophores. **A.J. Morris**

2:30. Examining effects of surface chemistry on quantum dots and nanocrystal films with time-resolved techniques. **A.B. Greytak**

2:50. Effect of lithium electrolyte concentrations on molecular structure, motions, and their impact on macroscopic properties. **D.G. Kuroda**

Durham Convention Center
Grand Ballroom I

Organic Chemistry Research and Development Poster Session

Cosponsored by ORGN
D. A. Canelas, K. C. Glasgow, *Organizers*

1:20 - 3:20

Poster Session.

101. Discovery and development of benzothiophene ketones as STING agonists [Poster Board #101]. **T.J. Henderson**, J.P. Jewell, M.D. Altman, A. Buevich, B. Cash, W. Chang, M. Childers, J. Cumming, A. Haidle, C.A. Lesburg, J. Lim, M. Lu, R. Otte, J. Piesvaux, G. Schroeder, B.W. Trotter, D.F. Wyss, D.J. Bennett

102. Development of ¹⁵N-labeled probes for hyperpolarized magnetic resonance imaging of γ -glutamyl transferase (GGT) activity [Poster Board #102]. **E. Minerali**, H. Park, Q. Wang

103. Chiral pool approach to the asymmetric synthesis of abyssomicin C: A gateway to analog synthesis and biological evaluation [Poster Board #103]. **A. Guerra, C. Walker**, N.P. Onuska, T.R. Jones, J.G. Pierce

104. Evaluating the scope and selectivity of the C-H borylation of thioethers [Poster Board #104]. **J. Myers**

105. Exploring structure activity relationships of G-protein biased kappa opioid receptors [Poster Board #105]. **K.S. Taylor**, H. Ma, R. Russo, V. Dang, L. Bohn, J. Aubé

106. Stereospecific synthesis of cyclobutanone derivatives via 1,2-rearrangements of cyclopropanone adducts [Poster Board #106]. **J.E. Muir**, V. Lindsay

107. Visible light-controlled pH modulation in solution using a novel merocyanine based photoacid [Poster Board #107]. **R. Choudhury**

108. Telescoped, continuous preparation of rifapentine mitigating nitrosamine formation [Poster Board #108]. **E. Stryker**, A. Matthews, T. Yue, F. Gupton

109. Synthesis of spiro[2.3]hexan-4-ones from stable cyclopropanone equivalents [Poster Board #109]. **B.M. Sulc**, J.E. Muir, V. Lindsay

- 110.** Synthesis of fully saturated Azepanes with all-carbon quaternary centers: Single-atom logic approach, asymmetric Schmidt rearrangement, and selectivity enhancement with HFIP [Poster Board #110]. **D.L. Hardee**
- 111.** Dihapto-coordination of pyridine and cyclic alkenes to a π -basic tungsten fragment for the organic synthesis of piperidyl-substituted Ritalin derivatives and functionalized five-, seven-, and eight-membered carbocyclic compounds [Poster Board #111]. **M.N. Ericson**, R. Stegner, A.Q. Meng, J.D. Dabbs, S.E. Megert, D.A. Dickie, W. Harman
- 112.** Azapeptoid synthesis: Determining amino acid compatibility during late-stage azaglycine alkylations [Poster Board #112]. **M. Carter**, M. Bowles, K. Cartrette, C. Proulx
- 113.** Organobismuth compounds as aryl radical precursors via light-driven single electron transfer [Poster Board #113]. **N. Chiappini**, E.P. Geunes, E. Bodak, R. Knowles
- 114.** Employing alkylation for the formation of α -Ketoalkynes [Poster Board #114]. **J. Jaramillo Gonzalez**, A. Yusufi, B.D. Feske
- 115.** Synthesis and SAR of antiviral compounds against HIV and HBV [Poster Board #115]. **T. Jones**, T.R. Lane, V. Makarov, S. Ekins
- 116.** Engineering monoterpene production in *Escherichia coli* by biosensor-guided high-throughput screening [Poster Board #116]. **E. Riser**, G.J. Williams
- 117.** Mechanistic and kinetic analysis of the oxidation of fluorinated silyl ethers [Poster Board #117]. **C. Rigsby**, A.G. Riccardi, A.L. Moser, M.L. Turley, S.K. Goforth, B.C. Goess
- 118.** Dearomatization-rearomatization of Pyridazinium ylides for the construction of new heterocycles [Poster Board #118]. **R. Tran**
- 119.** Progress towards the total synthesis of bisleuconothine A [Poster Board #119]. **H.C. Pageot**, A. Cholewczynski, J.G. Pierce
- 120.** Design and synthesis of testosterone conjugated DNA-damaging agents for cancer chemotherapy [Poster Board #120]. **M. Volety**, **E.G. Oettinger**, **J. Torres**, **N. Mendoza**, A. Frampton, S. Varadarajan
- 121.** Synthesis and self-assembling properties of a series of 4,6-p-fluorobenzylidene acetal 3-O-carbamate derivatives of D-glucosamine [Poster Board #121]. **H.A. Hisojo Romero**, G. Wang
- 122.** Dearomative cyclopropanation of electron-deficient heteroarenes using sulfones as carbene equivalents [Poster Board #122]. **C. Teeple**s, S.M. Wilkerson-Hill
- 123.** Synthesis and optical properties of donor- π - acceptor fluorophores containing 1,3-Indane dione moiety [Poster Board #123]. **Z. Gul**

- 124.** Structure-based discovery of psychedelic-inspired therapeutics [Poster Board #124]. **T. Kelly, J.G. Pierce**
- 125.** A blast from the past: Showcasing Evan's NMR method to measure magnetic susceptibility [Poster Board #125]. **J. Knoop, J.R. Alston**
- 126.** Nickel-catalyzed stereoselective synthesis of α -chiral amines through dicarbofunctionalization of 1,3-dienes [Poster Board #126]. **D. Mickles**
- 127.** State of generative AI in chemistry: Review of retrosynthesis [Poster Board #127]. **J. Park**
- 128.** Discriminating alcohol reactivity through reagent control: A model study on the alkylation of methyl 5-bromo-1H-indazole-3-carboxylate [Poster Board #128]. **L. Juarez, P. Wiget, P. Lu, W. Zhang, R. Krishnan, P.L. Kotian**
- 129.** Synthesis and gelation properties of a series of 3-O-carbamate derivatives of D-glucosamine [Poster Board #129]. **R. Chen, G. Wang**
- 130.** Concise synthesis of *N*-aryl benzimidazoles as small molecule activators of the human E3 ubiquitin ligase Nedd4-1 [Poster Board #130]. **H.S. DeHaan, D.G. McCafferty**
- 131.** Design and synthesis of cyanonilutamide conjugated DNA damaging agents targeting prostate cancer cells [Poster Board #131]. **K. Smith, M. Volety, M.Q. Schoppa, C. Agee, C. Leitz, A. Frampton, S. Varadarajan**
- 132.** Biocatalytic aza-Michael addition of aromatic amines to enone using α -amylase in water [Poster Board #132]. **S. DUTT**
- 133.** Synthesis of 4,6-O-(*p*-chlorobenzylidene) acetal-functionalized D-glucosamine carbamate derivatives and their applications [Poster Board #133]. **D.W. Wynn**
- 134.** Selective inhibition of UGDH with a series of novel peptide and peptoid analogs [Poster Board #134]. **K.E. Witte, S. Harrelson, E. Allego, C. Davern, E.J. Warner, C. Proulx, J.J. Barycki, M.A. Simpson**
- 135.** The chemoselective oxidation of thiols to disulfides using Bobbitt's salt [Poster Board #135]. **S. Weierbach**
- 136.** Nitroxide-mediated aerobic oxidation of 1-hexanol: Control of product selection via oxidation conditions [Poster Board #136]. **J.T. Dang, M.S. Ward, H.J. Schanz**
- 137.** Facile Synthesis of 1,4,2-Oxothiazols *via* MnO₂ Mediated Cyclization [Poster Board #137]. **A. Valdes, B. Cipriano, J.G. Pierce**
- 138.** High throughput experimentation at the University of Delaware [Poster Board #138]. **J. Sampson**

139. Determining optimum practical amounts of base to add to primary and secondary amines during protection reaction [Poster Board #139]. **K. McCrossin**, D.V. Liskin

140. Development of perinucleolar compartment disruptors as specific anti-metastasis agents [Poster Board #140]. **P.S. Dhote**, J. Rayadurgam, F. Wang, R. Flax, I. Mancera-Ortiz, E. Freeman, P. Lam, S. Huang, J.J. Marugan, N. Southall, S. Patnaik, K.J. Frankowski

141. Phosphoric acid catalyzed synthesis of chiral lactams [Poster Board #141]. **J. Dean**, K.S. Petersen

142. Investigating amiloride-based small molecule recognition of positive-sense viral RNA regulatory structures [Poster Board #142]. **T. Luu**, K. Chopra, M. Zafferani, S. Suzuki, A.E. Hargrove

143. Sustainable synthesis of furfural-based hydrazones as potential biofilm inhibitors, and well-designed macrocycles for nanoplastic untangling in aqueous media [Poster Board #143]. **K. Murphy**

Durham Convention Center
Grand Ballroom I

Physical Chemistry: Theory Development and Experimental Frontiers Poster Session

Cosponsored by PHYS
D. A. Canelas, *Organizer*

1:20 - 3:20

144. Modulating the driving force of naphthalene diimide excited-state PCET reactions [Poster Board #144]. **J. Mansergh**, J. Zhu, R. Liu

145. Predicting NMR relaxation and diffusion constants using molecular dynamics simulations: Applications to NMR interface studies [Poster Board #145]. **J. Simonpietri**, T.K. Meldrum

146. Microwave spectrum and analysis of 2,5-difluorophenol [Poster Board #146]. **G. Behie**, **E. Johnson**, **L. Morrison**, G.G. Brown

147. Microwave spectrum and analysis of 2,3,6-trifluorophenol [Poster Board #147]. **N. Ahmed**, **R. Sarkar**, **S. Vishnubhotla**, G.G. Brown

148. Microwave spectrum and analysis of 2,4,5-trifluorophenol [Poster Board #148]. **G. Dutta**, **B. Lahey**, G.G. Brown, **R. Bui**

- 149.** Novel Langevin models for fluorescent dye linker dynamics and the smFRET dynamic shift [Poster Board #149]. **D. Frost**, K. Cook, H. Sanabria
- 150.** Optimization of hyperpolarized pyruvate in ethanol water mixture using signal amplification by reversible exchange [Poster Board #150]. **M. Pike**, **E. Curran**, **A. Davidsson**, T. Theis
- 151.** Using high-order correlation functions to analyze noisy single-molecule data: A non-parametric and high time-resolution method [Poster Board #151]. **M. Dhar**, J.A. Dickinson, M.A. Berg
- 152.** Stark spectrometer for isomer separation and detection [Poster Board #152]. **J. Sudha Sobhanakumar**, L. Duffy
- 153.** Charge carrier dynamics in single conjugated polymer chain [Poster Board #153]. **M. Lei**
- 154.** TD-DFT triplet instabilities of iron-(II) polypyridine dyes [Poster Board #154]. **M. Rutledge**, G.M. Curtin, E. Jakubikova
- 155.** Theoretical rovibrational spectroscopy of magnesium Tricarbide - multireference character thwarts a full analysis of all isomers [Poster Board #155]. **D.A. Agbaglo**, Q. Cheng, R.C. Fortenberry, N.J. Deyonker
- 156.** Photophysical Studies and nitroaromatic sensing associated with the porphyrinic metal-organic framework PCN-222 [Poster Board #156]. **J.T. DeMatteo**, R.W. Larsen
- 157.** Adaptive basis sets and bond-centered basis functions for electronic structure calculations on quantum devices [Poster Board #157]. **P.B. Hogsed**, G.M. Curtin, E. Jakubikova
- 158.** Electroanalytical and negative ion photoelectron spectroscopic studies of P-benzoquinone radical anion, 1,4-naphthoquinone radical anion, and their deprotonated derivatives [Poster Board #158]. **N. White**, K. Workman, J. Moldenhauer, W.K. Gichuhi
- 159.** Direct, long-range electrostatic embedding with DFT-based QM/MM/PME: Energy and forces [Poster Board #159]. **J.P. Pederson**, J.G. McDaniel
- 160.** Hydrocarbon separations in porous materials: The role of polarization in modeling binding sites [Poster Board #160]. **M. Mulcair**, B. Space
- 161.** Characterizing the diffusion of select natural oils into wax systems with transmission Fourier-transform infrared spectroscopy [Poster Board #161]. **C. Mitchell**, T. Gregory, M. Higgins, S.W. Huffman
- 162.** Cyanoindene isomers: Predicted negative ion photoelectron spectra, singlet-triplet splittings, and isomer-specific thermochemical values [Poster Board #162]. **D.N. Koku Hannadige Abeysooriya**, K. Workman, J.A. Dupuy, W.K. Gichuhi

163. Modeling sorption in a dispersion dominated environment [Poster Board #163]. **L. Ritter**, B. Tudor, A. Hogan, T. Pham, B. Space

164. Demonstrating the relevance of many-body van der Waals through the coupled dipole method [Poster Board #164]. **M. Mostrom**, A. Hogan, B. Space

Durham Convention Center
Meeting Room 3

Chemistry Education Research and Practice

Cosponsored by CHED
S. L. Johnson, *Organizer*

1:30 Introductory Remarks.

1:35. General Chemistry instructors' perceptions on assessment questions targeting Le Chatelier's principle being used in exam/midterms, homework, and/or in-class activities. **E. Kable**, Y. Wang, L. Shi, M.N. Stains

1:50. Diffusion experiment based on the lower explosion limit of solvents. **J.W. Hall**, J. Guy, B. Tutkowski

2:05. Mentoring at-risk students in large enrollment General Chemistry 1. **M. Sumner**

2:20 Break.

2:30. Synthesis of Arylpropionic acids via carboxylation of Arylacetylenic Grignard reagents. **R. Okoth**

2:45. Classroom management support for teaching assistants: Building an engaging learning environment. **J. Alewine**, S. Stefl, J.L. Brumaghim

3:00. Peer-to-peer chemical safety education through the student-led joint safety team's curated resources. **B.L. Bresnahan**

Durham Convention Center
Meeting Room 4

Coordination Chemistry, Synthesis, Characterization and Reactions

Cosponsored by CATL, INOR and ORGN
Financially supported by Coastal Georgia Local Section
W. E. Lynch, *Organizer*

1:30 Introductory Remarks.

1:35. Synthesis and characterization of mixed valent {FeFeFe}¹⁹ EMACs with short Fe-Fe bonds. **G. Guillet**, J.E. Bates, X. Chen, K.Y. Arpin

1:55. Flexible linear tetracuprous arrays and large Cu^I clusters as blue-and green/yellow-light emitters. **M. Stollenz**, J. Arras, A. Calderón-Díaz, S. Lebendkin, S. Gozem, N. Bhuvanesh, C. McMillen

2:15 Break.

2:25. Dioxygen chemistry of mononuclear manganese-porphyrins and copper chelates: Individual and cooperative reactivities. **S. Hematian**, F. Tuglak Khan, D.S. Porter

2:45. Photolysis of Oxo-bridged heme/copper assemblies for production of oxidative intermediates: A combined experimental and theoretical approach. **F. Tuglak Khan**, S. Hematian

THURSDAY EVENING

Durham Convention Center
Grand Ballroom I

Transformation Products of Emerging Contaminants: What Are They, Where Are They, And How Do We Find Them? Poster Session

Cosponsored by ENVR
A. Brennan, D. Macmillan, *Organizers*

5:00 - 7:00

101. The US-EPA Chemical Transformations Database (A novel web application for storage, presentation, and comparative analysis of chemical transformations) [Poster Board #101]. **A. Edelman-Muñoz**, C. Tebes-Stevens, L. Shields, I. Thillainadarajah, B. Meyer, E.J. Weber, R. Kolanczyk, A. Williams

102. Targeted and non-targeted screening for seasonal environmental contamination levels in Durham, NC surface waters using liquid chromatography-high resolution mass spectrometry [Poster Board #102]. **J. Apoian**, N. Hale, P.L. Spence, O.E. Christian, C. Gerald, I. Walker Karega

103. Quantum chemical calculations of ingredients in hair dye interacting with DNA bases [Poster Board #103]. **S. Arachchi**

104. Polymer associated chemicals released from HDPE and tire microplastics sourced from recycling facilities [Poster Board #104]. **K. Tober**, A. Grant, Z. Eastman, I. Walker Karega

105. Influence of nanoparticles surface on the activity of the antibiotics anchored at the interface [Poster Board #105]. **M.M. Sa'ed**, S. Tahmasebi Nick, S.O. Obare

106. PFAS degradation by nano zero valent aluminum [Poster Board #106]. **E. Hayden**, J.C. Poler

FRIDAY MORNING

Durham Convention Center
Junior Ballroom B

Southeastern Magnetic Resonance Conference (SEMRC)

Cosponsored by ANYL and PHYS
A. I. Smirnov, M. A. Ter Horst, *Organizers*

8:00 Introduction: Materials Session.

8:05. Understanding nanoconfinement and local molecular correlations in molecular and ionic transport media. **L.A. Madsen**

8:25 Q&A with Dr. Madsen.

8:35. EPR studies of phthalocyanines encapsulated in zeolites. **M.G. Bakker**, G. Rana, E. Wissman, A. Frederick, E.P. Iaia, J.W. Harris

8:50. Nanoparticle additives alter radical-driven degradation of oil lubricants: Spin-trapping EPR studies. **J. Matheny**, T. Smirnova, P. Bankaitis, R. Rana

9:05 Break, Next Session: Enzymes.

9:15. EPR studies of the enzymatic synthesis of the organometallic H-cluster of [FeFe] hydrogenase. **R.D. Britt**

9:35 Q&A with Dr. Britt.

9:45. Leveraging solution NMR-based ligand Dynamics Information for lead optimization. **P. Zhou**

10:00. Exploring the space of different reactions and different sites in enzymes to resolve select dynamical contributions to catalysis, by using multiple EPR approaches. **K. Warncke**, A. Ionescu, W. Li

10:15 Break, Next Session: New Methods and Instrumentation.

10:25. Neural net analysis of strongly coupled spin systems. **J.H. Prestegard**, J.N. Glushka, J.H. Grimes

10:45 Q&A with Dr. Prestgard.

10:55. Ultra-low-temperature (8 K) static NMR-DNP for metalloproteins and materials. **D. Doty**, S. Deese, J. Spitzmesser, G. Doty, D. Arcos, J. Staab, L. Holte, J. Doty, P. Ellis

11:10. ^{13}C -detected measurement of ^{13}C - ^1H RDCs using paramagnetic ion alignment. **A. Eletsky**, C. Huang, K. Moremen, J. Prestegard

11:25 Break.

11:35. Terahertz EPR spectroscopy using a 36-Tesla high-homogeneity series-connected hybrid magnet. **t. dubroca**, F. Mentink-Vigier, S. Hill, J. Krzystek

11:50. PBG resonators for pulsed EPR at W- and G-bands. **S. Milikisiyants**, A. Marek, A. Nevzorov, A.I. Smirnov

12:05. Chirp pulse magic as used for the mixing schemes of ^{13}C - ^{13}C , ^{15}N - ^{15}N , ^{13}C - ^{15}N , and ^1H - ^1H correlations. **S. Wi**, L. Frydman, W. Lee

Durham Convention Center
Junior Ballroom A1

Project SEED

Cosponsored by CHED
A. Mallia, *Organizer*

8:30 Introductory Remarks.

8:35. Eight weeks of Project SEED and a one-week drug discovery camp: Summer chemistry activities for high school students in the ACS Snake River local section. **D.L. Warner**

8:55. A CURE for underrepresentation in STEM: Getting high school students involved in research through adaptation of a course-based undergraduate research experience. **E. Reynolds**

9:15. Implementation of Project SEED in a small two-year college. **J.W. Hartman**

9:35. ACS project SEED student rotations in an undergraduate research program. **K. Dungey, B. Stein, W. Yang, J.A. Pienkos**

9:55. Getting high school students involved in research. **S.A. Fleming**

10:15 Intermission.

10:30. Project SEED at the University of Southern Mississippi. **D.S. Masterson**

10:50. Success and impact of the ACS project SEED Program at Georgia Gwinnett College. **A. Mallia, N.Y. Forlemu, S. Mwangela**

11:10. Louisiana Tech University's 2023 ACS project seed experience with cohort 1. **K. Ruddick, R. Beminiwattha, E. Castagnola, A. Moore, N. Wasiuddin, Y. Xiao**

11:30. Project SEED: North Carolina section of the American Chemical Society. **A. LOPES**

11:50. Training the next generation of analytical scientists with Project SEED through the detection of fluorinated persistent organic pollutants. **J.T. Shelley, T. Jones, J.L. Danischewski, J. Viggers**

12:10 Concluding remarks.

Durham Arts Council
Duke Rehearsal Hall

Single-molecule Dynamics in Complex Chemical and Biological Systems

Cosponsored by ANYL, BIOL, BIOT and PHYS
A. Gahlmann, K. Welsher, *Organizers*

8:30 Introductory Remarks.

8:35. Single-molecule dynamics of membrane-proximal actin in live B cells. **J. Flanagan-Natoli, A. Decker, A. Stoddard, S. Veatch**

8:55. High-confidence single-molecule detection of nucleic acid biomarkers. **K.M. Wijesinghe, J. Harrell, S. Dhakal**

9:15. Integrating light sheet illumination and microfluidics for 3D single-molecule super-resolution mammalian cell imaging. G. Gagliano, N. Saliba, **A. Gustavsson**

9:35. Long axial range double-helix point spread functions for 3D single-molecule super-resolution imaging in mammalian cells. **Y. Nakatani**, A. Gustavsson

9:50. Tracking of specific genomic loci in three dimensions with high spatiotemporal resolution. **A. Raterink**, R. Ghosh, M. Nguyen, A. Gustavsson

10:05 Break.

10:15. Single-fluorogen imaging reveals the nanoscale structure of beta-sheet assemblies and biomolecular condensates. T. Wu, W. Zhou, M. Farag, M.R. King, C.L. O'Neill, T. Ding, O. Zhang, J.S. Rudra, R.V. Pappu, **M.D. Lew**

10:35. Guiding proteins through conformational landscapes using anharmonic low-frequency vibrations. S. Mondal, M.A. Sauer, **M. Heyden**

10:55. Investigating the conductance distributions of single-molecule junctions using ab initio molecular dynamics. **M. Curry**, A. Wunschel, S. Roy

11:10. Developing a bright and solvatochromic BODIPY fluorescent probe for functional super-resolution imaging of cell membrane. **Y. Liu**, J. Chen, Y. Zhang

Durham Convention Center
Grand Ballroom I

Undergraduate Poster Session

Cosponsored by CHED
J. A. Feducia, K. C. Glasgow, *Organizers*

8:30 - 10:30

101. Impact of ultraviolet light on aggregation-induced fluorescence of rhodamine B amide derivatives [Poster Board #101]. **M. Hill**, D. Wright, K.H. Fogarty, P. Lundin

102. Analysis of self-assembly in acridine orange and cucurbit[n]uril systems by atomic force microscopy [Poster Board #102]. J. Miller, **M.R. McPhail**, F.A. Khan

103. Real time detection of G-type nerve gas agents using a rhodamine-B based sensor [Poster Board #103]. **E. Norman**, A. Weerasinghe

- 104.** Cyclic voltammetry investigation of redox chemistry of rhodamine B amide derivatives [Poster Board #104]. **D. Wright**, K. Fogarty
- 105.** Optimizing pretreatment strategies for the SERS-based identification of microscopic samples from early American oil paintings [Poster Board #105]. **M. Martin, B. Steinman**, K.L. Wustholz
- 106.** A kinetic analysis of prodrug activation by β -lactamase enzymes [Poster Board #106]. **A. Dale**, A.M. Duda, K.J. Franz
- 107.** Investigating RNA G-quadruplex:small molecule recognition through the scope of RNA/DNA selectivity [Poster Board #107]. **N.I. Montalvan**, J.G. Martyr, E. Swanson, A.E. Hargrove
- 108.** Evaluation of the laccase-like multi-copper oxidase from *Paenibacillus gluconolyticus* for non-natural biocatalysis [Poster Board #108]. **C. Creed**, E. Reynolds
- 109.** Investigating photocontrol of SAM-II riboswitch conformations through azobenzene small molecules [Poster Board #109]. **G. Wang**, D. Santana, A.E. Hargrove
- 110.** Exploring conformational composition in small peptides [Poster Board #110]. **J.E. Pieper**, L.E. Buchanan, S. Parnham, M.W. Giuliano
- 111.** The somatostatins and hydrophobic effects in cyclic peptides [Poster Board #111]. **J.C. Herring**, S. Parnham, M.W. Giuliano
- 112.** Rational design of mutations to expand the substrate scope of the thiamine-dependent enzyme SucA [Poster Board #112]. **A.C. Girard**, E. Reynolds
- 113.** Tailorable analgesic release from biodegradable poly(ester urea) nanofibers for controlled drug delivery in combat wound management [Poster Board #113]. **K. Coaker**, C. Dziewior, M. Becker
- 114.** Gluten free beer produced from buckwheat and millet [Poster Board #114]. **L. Rose**, D. Budner
- 115.** Optimization of the production and expression of recombinant human adrenodoxin in *escherichia coli* [Poster Board #115]. **K.R. Provost**, M. Reddish
- 116.** Selection of bacteria to grow on plastic with increased crystallinity [Poster Board #116]. **J. Reed**, M.K. Lorenger, T.D. Gruber
- 117.** Genetic modification trials of *I. sakaiensis* through conjugation [Poster Board #117]. **C.R. Salazar**, M.K. Lorenger, T.D. Gruber

118. Purification and characterization of a novel alcohol dehydrogenase from *Commensalibacter intestini* [Poster Board #118]. **E. Francisco**, B.E. Christian

119. Structural effects on aromatase inhibition for the treatment of estrogen receptor-positive breast cancer [Poster Board #119]. **S. Land**

120. Investigation of geographical origin of honey using measures of antioxidant potential [Poster Board #120]. **S. Zeballos**, D. Budner

121. Utilizing boron nitride nanomaterials for water remediation [Poster Board #121]. **A. Sheffield**, J.G. Clar

122. Investigation of zinc and iron in wildflower honey [Poster Board #122]. **S. Simpson**, D. Budner

123. Getting undergraduate students involved in microplastic research [Poster Board #123]. **K. Carnes**, E. Stewart, R. Meeks, C. McCloy, S. Lynch, C. Reagan, E. Crisp, J. Burgess

124. Experimental and theoretical investigations on metal-organic complexes for the capture of hydrogen sulfide [Poster Board #124]. **C. Rodgers**, P.N. Bobadova, C.M. Wallen

125. Coordination of protic oxygen and sulfur species with metal-sulfonamidate complexes via second-sphere hydrogen bonding [Poster Board #125]. **M. Hern**, C.M. Wallen

126. Application of ionic metathesis reactions towards synthesis of photoswitchable and drug-delivery bio-based ionic liquids [Poster Board #126]. **H. Miller**, J.J. Pajski

127. Effect of complexation of heavy metals on removal by magnetic nanoparticles [Poster Board #127]. **C. O'Brien**, **G. Balkey**, K.M. Mullaugh

128. Effects of altered ligand structure on the coordination of protic sulfur species to sulfonamidate metal complexes with second sphere hydrogen bonding [Poster Board #128]. **R.R. Foley**, C.M. Wallen

129. Zinc oxide as a potential transesterification catalyst in PDMS vitrimer composites [Poster Board #129]. **Y. Hu**, B. El-Zaatari

130. Development of first-row transition metal complexes with redox-active catecholamine ligands and their corresponding reactivity [Poster Board #130]. **Z. Wang**, A. Yu, J. Bacsa, C.E. MacBeth

131. Exploring second-sphere hydrogen bonding in metal-organic coordination complexes for the capture of hydrogen sulfide [Poster Board #131]. **R. Byrd**, C.M. Wallen

132. Factors that influence the removal of Fe²⁺ ions from aqueous solution using sodium alginate hydrogels [Poster Board #132]. E. Ingle, **J.L. Hawk**

- 133.** Enzymatic cross-coupling of carbonyl compounds and alkyl halides: Crossing into new territory with thiamine-dependent enzymes [Poster Board #133]. **R.C. VanWinkle**, E. Reynolds
- 134.** Synthesis of Phenpropylamines [Poster Board #134]. **J. Baek**, T.J. Barker
- 135.** Pd-catalyzed cross-coupling of alkyl bisboronic esters [Poster Board #135]. **P. Scott**, T.J. Barker
- 136.** Optimization of the route to flinderole core [Poster Board #136]. **K. Watts**, B. Wakefield
- 137.** Synthesis of phenyl-containing phidianidine analogs [Poster Board #137]. **H. Higgins**, T. Ghering, S. Ross, A. Tingler, **B. Wakefield**
- 138.** Synthesis of furan-containing phidianidine analogues [Poster Board #138]. **T. Berry**, T. Ghering, H. Higgins, S. Ross, A. Tingler, B. Wakefield
- 139.** Attempted syntheses of the flinderole core [Poster Board #139]. **A. Pettijohn**, C. Romain, B. Wakefield
- 140.** The effect of water ionic chemistry on the bioactive phenolic compounds in kombucha [Poster Board #140]. **S. Disselkoen**, **D. Budner**
- 141.** Effects of substituents and reaction conditions on the oxidation kinetics of benzyl silyl ethers [Poster Board #141]. **M.L. Turley**, A.G. Riccardi, M. McKenna, C. Rigsby, A.L. Moser, B.C. Goess, S.K. Goforth
- 142.** Optimization of a pedagogical multistep synthesis involving alcohol halogenation and Williamson ether synthesis [Poster Board #142]. **K.J. Kellar**, N.M. Woodlief, S.K. Goforth
- 143.** Oxidation of TBS, TBDPS, and TMS benzyl ethers to form silyl benzoates [Poster Board #143]. **A.L. Moser**, A.G. Riccardi, R.W. Peterson, C. Rigsby, M.L. Turley, B.C. Goess, S.K. Goforth
- 144.** Preparation, characterization and Conformational Analysis of cyclopropyl-chloromethyl-difluorosilane [Poster Board #144]. **J. Bethke**, O.R. Hawk, A. Davies, V. Sablinskas, G. Grubbs, G.A. Guirgis
- 145.** Comparative *in silico* study of the toxicology of novel synthetic opioids using multivariate statistical methods [Poster Board #145]. **K. Hubbard**, A. Bruni, E.G. Geraldo de Campos
- 146.** Computational modeling of a series of 8(meso)-pyridyl-BODIPYs [Poster Board #146]. **D. Goliber**, d. LaMaster, E. Hernandez, P.N. Bobadova
- 147.** Predicting aryl carbene singlet-triplet energy differences beyond the random phase approximation [Poster Board #147]. **J. McKeon**, S. Work, J.E. Bates

- 148.** Computational modeling of a series of unsymmetric bis(bf₂) BODIPYs: Boppys [Poster Board #148]. **S. Al Horani, M. Al Horani**, P.N. Bobadova
- 149.** Kinetic analysis of static motifs in flavin-based electron bifurcating enzymes provides insight to structural basis for efficient energy transducing electron transfer [Poster Board #149]. **W. Milhizer**, K. Terai, D.N. Beratan
- 150.** Using molecular dynamics to simulate covalent labeling experiments [Poster Board #150]. **W.C. Huffman**, B. Perez-Soto, S. Lindert
- 151.** Targeting selective transmission of constructive J-couplings in SABRE-SHEATH hyperpolarization [Poster Board #151]. **R.S. Raman**, J. Lindale, W.S. Warren
- 152.** Estimation of nanoparticle exposure via dermal contact: A variety of coated surfaces [Poster Board #152]. **G. Tolbert, R. Kolaitis**, J.G. Clar
- 153.** Student perceptions of learning in a senior level flipped forensic chemistry course [Poster Board #153]. **L. Sharman**, A. Chee-Awai, T. Legron-Rodriguez
- 154.** Chemistry for a sustainable future: An international NSF Research Experience for Undergraduates (REU) in the United Kingdom [Poster Board #154]. **T.A. Nile, A.G. Glenn**, N. Chiu, C. Cox, N. Dabney, F. Green, Z. Jackson, Z.S. Moore, G. Rich, K. Yard
- 155.** Identifying themes of students' sense of belonging in general chemistry [Poster Board #155]. **Z. Torres**, K. Muller, T. Legron-Rodriguez
- 156.** Exploring perceived student engagement in a flipped classroom, senior-level forensic chemistry course [Poster Board #156]. **A.C. Chee-Awai**, L. Sharman, T. Legron-Rodriguez
- 157.** Development and evaluation of audible titration modules: Chemistry learning for visually impaired students [Poster Board #157]. **C. Fine**, C. Devera, R. Dabke, K.S. Taylor
- 158.** Studying hydrogen quantum tunneling across a plant lipoxygenase library in a biochemistry course-based undergraduate research experience (CURE) Laboratory [Poster Board #158]. **Y. Ly**, K. Sagrero, E. Brinkley, J.P. Walker, A.R. Offenbacher
- 159.** Creation of a novel and synthesizable electrochromic device from nanosheets [Poster Board #159]. **R. Martens**, T. Anglin
- 160.** Facile procedure of cost effective Bi doped SnO₂ catalysts for the CO₂ electroreduction reaction [Poster Board #160]. **O. Tercioglu**, T.C. Anglin
- 161.** Computational design and synthesis of a CLIPTAC molecule for the treatment of Alzheimer's disease by tau degradation through the ubiquitin-proteasome system [Poster Board #161]. **o. avery**, M. Bruno, T. Anglin

162. Photochemical study of vitamin D Field in supramolecular host systems [Poster Board #162]. **E. Baker**, S. Gupta

163. Mechanistic elucidation of nanomaterial-enhanced first-generation biosensors using sweep voltammetry [Poster Board #163]. **J.S. Kaplan**, A. Wemple, M.C. Leopold

164. Forensic discrimination of EDTA in dried blood using attenuated total reflectance spectroscopy [Poster Board #164]. **H. Herndon**, **A. Howell**, J. McCutcheon

Durham Convention Center
Meeting Room 3

Structure-Based Drug Design

Cosponsored by MEDI and ORGN
R. J. Bienstock, *Organizer, Presiding*

8:45 Introductory Remarks.

8:50. Hit discovery using docking enriched by generative modeling (hidden gem): A novel computational workflow for accelerated virtual screening of ultra-large chemical libraries. K. Popov, **J. Wellnitz**, T. Maxfield, **A. Tropsha**

9:05. Structure-based generative AI for *de novo* drug design: PIM-1 Kinase case study. **R. Arora**, M. Medcalf, M. Monson, A. Kriukova, P. Jacquemard, A. Martinez, S. Sautet, A. Denis, M. Jusot, C. Housseman, N. Devaux, S. Labouille, B. Atwood, Y. Gaston-Mathe, Y. Lamotte, Q. Perron, N. Do Huu, B. Hoffmann

9:20. Using molecular dynamics to produce an ensemble of protein conformations to yield more biologically relevant docking results. **R.J. Bienstock**, R. Hara, A. Kayal, S. Firth-Clark, N. Kidley

9:35. Design and discovery of MRTX0902, a potent, selective, and orally bioavailable clinical SOS1 inhibitor. **J. Ketcham**, S. Khare, V. Bowcut, D. Briere, A.C. Burns, R. Gunn, J. Haling, A. Ivetac, J. Kuehler, S. Kulyk, J. Laguer, D. Lawson, K. Moya, N. Nguyen, L. Rahbaek, B. Saechao, C. Smith, N. Sudhakar, N. Thomas, L. Vegar, T. Scattolin, D. Vanderpool, X. Wang, L. Yan, P. Olson, J. Christensen, M. Marx

9:50 Break.

10:00. First covalent small-molecule ligands for the triple Tudor domain of SETDB1. **M. Uguen**, D. Shell, M.S. Stashko, F. Li, L.E. Herring, J.L. Norris-Drouin, S. Ackloo, K.H. Pearce, S.V. Frye

10:15. Inhibition of an inflammatory cytokine with small molecule inhibitors for the suppression of breast cancer metastasis. **D.L. Warner**

10:30. Development of potential drug candidates for cancer therapy using molecular hybridization and rational drug design approaches. **S.S. Panda**

10:45. Development of fungal-specific calcineurin inhibitors derived from FK506/520. **P.A. Dome**, A. Rivera, W. Lim, E. Park, M.J. Hoy, I. Spasojevic, S. Sun, A.F. Averette, S. Pina-Oviedo, P.R. Juvvadi, W. Steinbach, M. Ciofani, J. Hong, J. Heitman

11:00 Break.

11:10. Development of direct-acting antivirals against SARS-CoV-2. **A. Hossain**, P. Brown, T. Willson

11:25. Broad-spectrum cyclopropane-based inhibitors of coronavirus 3-CL proteases: Biochemical, structural, and virological studies. **C.S. Dampalla**, H.N. Nguyen, A.D. Rathnayake, Y. Kim, K.D. Perera, T.K. Madden, H.A. Thurman, A.J. Machen, M.M. Kashipathy, L. Liu, K.P. Battaile, S. Lovell, K. Chang, W. Groutas

11:40. Uncovering the mechanism of action of novel quaternary phosphonium disinfectant P6p-10,10. **C.A. Sanchez**, G. Vargas-Cuebas, K.P. Minbiole, W.M. Wuest

11:55 Closing Remarks.

Durham Arts Council
IBM Rehearsal Hall

Biochemistry Research and Development

Cosponsored by BIOL and BIOT

D. A. Canelas, *Organizer*

H. T. Kratochvil, E. Pieri, *Presiding*

8:55 Introductory Remarks.

9:00. De novo designed proton channels test mechanisms of proton selective transport. **H.T. Kratochvil**, L. Watkins, M. Mravic, N. Somberg, J. Thomaston, J. Nicoludis, L. Liu, M. Hong, G.A. Voth, W. DeGrado

9:15. Characterization of putative periplasmic binding proteins from *Thermotoga maritima*. **J.D. Dattelbaum**

9:30. Identification of protein networks for dynamic activation of hydrogen tunneling in lipoxygenases. **A.R. Offenbacher**

9:45 Intermission.

9:55. Copper-dependent peptide cyclase is responsible for diverse plant side chain cross-linked cyclopeptides. S. Lima, M. Pasquale, B. Ampolini, E. Underwood, C. Earp, T. Graf, I. Khedi, S. Hematian, **J.R. Chekan**

10:10. A new Cu(II) binding site in a bacterial protein with cupredoxin fold. **S. Banerjee**

10:25. Determining the effect of copper-binding cysteines on protein precipitation. **A. Robison,** G. Sturrock, M.C. Fitzgerald, K.J. Franz

10:40. Elucidating interactomes of iron-sulfur cluster trafficking proteins in *Escherichia coli*. **D. Reasons,** F.W. Outten

10:55 Intermission.

11:05. Photoactivated ruthenium-based anticancer prodrugs. **J.A. Pollock,** M.R. Norris

11:20. Small molecule targeting of *Streptococcus mutans* AgI/II to inhibit dual-species biofilm with *Candida albicans*. **S.E. Velu**

11:35. Targeting the PqsE-RhlR interaction with small molecules to inhibit quorum sensing in *Pseudomonas aeruginosa*. **J. Derringer,** I. Taylor

11:50. Unraveling the mechanisms behind the phototoxicity of anthracene in high ionic strength environments. **A. Ugboya,** K.B. Grant

Durham Arts Council
PSI Theatre

Inorganic Chemistry Research and Development

Cosponsored by INOR
D. A. Canelas, K. C. Glasgow, J. M. Harrington, *Organizers*

9:00 Introductory Remarks.

9:05. Development of phosphorus extrusion chemistry. **B. Wicker**

9:20. Improving co-electrocatalytic activity for CO₂ reduction at lower overpotentials through redox mediator tuning and catalyst design. **A.G. Reid**, M.E. Moberg, C. Koellner, S.L. Hooe, K.R. Baugh, D.A. Dickie, C.W. Machan

9:35. Surface ligands shifts the semi-hydrogenation selectivity over palladium catalysts. **W. Zhang**, N. Zheng

9:50 Break.

10:00. Insertion of isocyanide into Re (III) Complex: Formation of η^1 and η^2 rhenium complexes. **A.K. Adegboyega**, L. Ribeiro Gouveia, E.A. Ison

10:15. Mechanistic insight into the reaction of CO with oxorhenium and nitridorhenium hydrides: Ligand and substituents effect on geometry and reactivity for the CO insertion in rhenium hydride and formyl bonds. **J. Borketey**, E.A. Ison

10:30. Antiferromagnetic chain chalcogenides as hosts of non-collinear spin textures. I. Campbell, J. Clark, **M. Shatruk**

10:45. Structure directing agents for the targeted synthesis of salt-inclusion materials. **G. Morrison**, H. zur Loye

11:00 Break.

11:10. Magnetic phase boundary mapping of AT₆Ge₆ structures (A = Y, Zr; T = Fe, Co) with kagomé layers of transition metal atoms. **V. Li**, M. Shatruk, M. Adams

11:25. Hold my purse! Establishing the fundamentals of spin-crossover behavior and catalysis in single-chain nanoparticle metallopolymer. C. Solomon, M. Ukiwe, **D.C. Ashley**

11:40. The magnetism of 2D ferromagnetic Fe₃GeTe₂ nanosheets functionalized with TCNQ molecules. **G. Sasi Kumar**

11:55. Catalytic behavior of NU-1000 grafted with organometallic catalysts. **L.J. Barrios**, V. Montiel-Palma, C. Secrist

Durham Convention Center
Junior Ballroom A3

Methods and Applications of High-Resolution Mass Spectrometry

Cosponsored by ANYL and ENVR
J. P. McCord, E. M. Ulrich, *Organizers*

9:00 Introductory Remarks.

9:05. Investigation of the sulfo-phospho-vanillin reaction for lipid sample normalization in untargeted LC-MS/MS quantitation as compared to conventional normalization techniques. **L.S. Bailey**, K.B. Basso

9:20. New adaptations of old tools: Development of a rapid HPTLC-HRMS based screening platform for metal-specific metallophore production by marine bacteria. **W.K. Strangman**

9:35. Maximized spatial information and minimized acquisition time of top-hat IR-MALDESI-MSI of zebrafish using nested regions of interest (nROIs). **A. Joignant**, M. Ritter, K. Knizner, K. Garrard, S.W. Kullman, D.C. Muddiman

9:50 Break.

10:00. Investigating the role of disulfide bond formation in tardigrade cryptobiosis. **E. Stair**, D. Kolling, L. Hicks

10:15. Exploring the role of post-translational modifications in tardigrade cryptobiosis. **S. Balboa**, D. Kolling, L. Hicks

Durham Convention Center
Junior Ballroom C

Organic Chemistry Research and Development

D. A. Canelas, K. C. Glasgow, *Organizers*
S. Harwood, *Presiding*

9:00 Introductory Remarks.

9:05. Mild, diastereoselective reduction of sulfinyl imines mediated by a zirconium hydride. **S. Harwood**, A. Aloiau, B. Bobek, K. Caddell-Haatveit, K. Pearson, A. Watkins, J. Ketcham, C. Smith, M. Marx

9:20. Development of a photocatalytic Suzuki-Miyura cross-coupling mediated by a Co(III) complex. **C.A. Bruno**, J.M. Bray, K.M. Lambert, J. Vredenburg

9:35. Bimolecular formation of piperazines via organic photoredox-catalyzed α -carbonyl radical addition to imines. **A. Boley**

9:50. Mild enantioselective reductive functionalization of amides via titanium multicatalysis. **J.A. Wilt**, G. Gutierrez

10:05 Break.

10:15. Palladium-catalyzed regiodivergent three-component carboamination of 1,3-dienes. **X. Ma**

10:30. Palladium-catalyzed trans-selective synthesis of spirocyclic cyclobutanes using α,α -Dialkylcrotyl- and allylhydrazones. **I. Eckart-Frank**, S.M. Wilkerson-Hill

10:45. A dearomative (3+2) cycloaddition enabled by chromium photocatalysis. **A. Smith**, B.K. Gall, E.M. Ferreira

11:00. Ru(II)-catalyzed transient directing group-assisted intermolecular asymmetric hydroarylation of bicycloalkenes. **N. Udayanga**

11:15 Break.

11:25. *N*-heterocyclic carbene pincer complex Re: Synthesis, structure, and catalytic activities for C-C cross-coupling of ketones, alcohols and one-pot synthesis of quinolines. **H. Pham**, B. Donnadieu, T. Hollis

11:40. Enantioselective amino- and oxycyanation of alkenes via organic photoredox and copper catalysis. **S. Qian**, T.M. Lazarus, D.A. Nicewicz

11:55. Photoredox-enabled total synthesis of Bisdehydrostemoninine and Bisdehydroneostemoninine. **N.R. Akkawi**, D.A. Nicewicz

Durham Convention Center
Junior Ballroom A2

Physical Chemistry: Theory Development and Experimental Frontiers

Cosponsored by PHYS
D. A. Canelas, *Organizer*
R. Lavrich, *Presiding*

9:00 Opening Remarks.

9:05. Inductive effects on intramolecular hydrogen bond strength examined by high resolution Fourier-transform microwave spectroscopy and MP2/6-311G++(d,p) calculations. K. Yap, K.D. Krantzman, **R. Lavrich**

9:20. Mixed organic valence states in quinone and dinitrobenzene radical anions: A combined electrochemical and negative ion photoelectron spectroscopy study. **W.K. Gichuhi**

9:35. Capturing *syn*-Propanethial-S-oxide. **C. Cadena**, C. Roberts

9:50 Break.

10:00. Development of a new L-shaped FT-microwave spectrometer with high-resolution and broadband capabilities. R. Rajapaksha, **M. Swann**, C. Miller, D. Duvall, R.M. Gurusinghe

10:15. Classical correlation model for surface enhanced infrared absorption and surface enhanced Raman spectroscopies. **Y. Gao**, D.E. Aspnes, S. Franzen

10:30. Predicting the reactions of the Lewis acid gases SO_x and NO_x with group IV and group VI transition metal oxide nanoclusters. **Z. Lee**, N.A. Joyner, L.A. Flores, M.S. Blair, D.A. Dixon

10:45. Accelerating crystal structure prediction using a machine-learned force-field for drug-like molecular crystals. I. Migliaro, **Z. Beckwith**

11:00 Break.

11:10. Unraveling the biomechanical properties of dystrophin's central rod domain: Implications for mechanosensing and therapeutic strategies in Duchenne muscular dystrophy. **T. Sizemore**, R. Bernardi, D. Gomes, P.S. Gomes

11:25. Mechanistic insights into tyrosine oxidation revealed by fast-scan cyclic voltammetry. **J. Todorov**, G.S. McCarty, L.A. Sombers

11:40. Homogenous and heterogenous electrode effects on conductance of single-molecule junctions containing chalcogen-terminated aliphatic and aromatic bridging molecules. **D. Landrie**, K. Reynolds, S. Roy

11:55. Surface chemistry from electron irradiation of schreibersite (Fe₂Ni)_p. **T. Davis**

Durham Arts Council
Adaron Hall

Ultrafast and Nonlinear Spectroscopy

Cosponsored by ANYL

Financially supported by Light Conversion, Ultrafast Systems, and Phase Tech Spectroscopy

E. Ghadiri, *Organizer*

L. Wang, *Presiding*

9:00 Introductory Remark.

9:05. Investigating peptide structure and polymorphism with 2D IR spectroscopy. **L.E. Buchanan**

9:25. Real-time propagation approach to TDDFT. **Y. Kanai**

9:45. Frequency combs as the route to the spectroscopic trifecta: High time resolution, high frequency resolution, and high sensitivity. **M.A. Reber**, N.D. Cooper, W.M. Jones, T. Eliason, J. Zhan

10:05 Intermission.

10:15. Electrode induction effects on the dynamics and reactivity of adsorbed molecules. **T. Lian**

10:35. Advancements in non-linear optical switching materials: Emerging solid-state metal halides. **L. Quan**

10:55. Phase-free, phase-resolved second harmonic generation studies of charged interfaces. **P.E. Ohno**

Durham Convention Center
Junior Ballroom D3

Chemistry Education Research: Undergraduate Student Research Symposium

Cosponsored by CHED
N. Lapeyrouse, C. Randles, *Organizers*

9:30 Introduction.

9:35. Help! I'm "diene": Interactive games to survive organic chemistry. **M. Canicatti**, S.M. Landge, C.R. Whitlock

9:50. Passing the first semester of general chemistry: A support course to mitigate student success barriers. **A. Gay**, A. Howell, J. Perry Cecile

10:05. Student feedback on their experience using mastery paths in general chemistry. **A. Cinque**, J. Miller, T. Legron-Rodriguez, N. Lapeyrouse

10:20. Contributions to an undergraduate research experience. **A. Allen**

10:35 Break.

10:45. Examining student perspectives of canvas mastery path adaptive learning modules. **J. Miller**, A. Cinque, N. Lapeyrouse, T. Legron-Rodriguez

11:00. Experiences of marginalized women pursuing doctoral degrees in chemistry: The critical role of recognition. **R. Ahmed, E. Cieza**, T. Jones, J.M. Pratt, M. Popova

11:15. Investigating student stress increases when exposed to biochemical visual representations by using galvanic skin response and working memory limitations. **G. Winslow**, C. Randles

11:30. Beyond VeSpR- the significance of conjugation in determining hybridization. **W. Lieber**, C.T. Cox

11:45 Closing Remarks.

Durham Convention Center
Junior Ballroom D2

Finding Your Pathway

Cosponsored by PRES and YCC
D. A. Canelas, K. C. Glasgow, *Organizers*

9:30 Introductory Remarks.

9:35. A day in the life of a professor at a research-intensive university. **F.A. Leibfarth**

9:55. My route in small molecule process research and development. **J. McCabe Dunn**

10:15. A career in cheminformatics at the US Environmental Protection Agency - serving the scientific community with Internet-based data. **A.J. Williams**

10:35. Finding Your Path...it just may be a lifelong journey!. **J.C. Giordan**

10:55 Panelist Q&A.

Durham Convention Center
Grand Ballroom I

Undergraduate Poster Session

Cosponsored by CHED
J. A. Feducia, K. C. Glasgow, *Organizers*

10:40 - 12:40

101. Electrophoretic studies of naphthoquinone-induced modification of lysozyme at various pH [Poster Board #101]. **L.R. Wooten**, J. Kim

102. Applications of differential sensing and LC-MS to seaweed classification and characterization [Poster Board #102]. **B. Ho**, D. Zamora-Olivares

103. Fluorescent sensing of melatonin by melatonin-based carbon dots [Poster Board #103]. **S. Kheterpal**, C.L. Colyer

104. Developing an IL-1 β electrochemical sensor and integrating with a fetal membrane on-a-chip [Poster Board #104]. **J. Martin**, H. Richards, O. Owens, G. Buckey, D.E. Cliffel

105. Caffeine and coffee by degree of roast: Sources of variation in reported data [Poster Board #105]. **R. Meeks**, H. Taylor, K. Carnes, P. Splichal, Z. Lindsay, J. Burgess

106. Differences in phototoxicity of menadione and plumbagin in the presence of reducing agents examined via DNA damage [Poster Board #106]. **S. Kannan**, K.B. Grant

107. Studying the loading efficiency and maintenance of protein activity after attaching them to magnetic nanoparticles using covalent bonds and non-specific adsorption [Poster Board #107]. **A. Angela**, T. Vasicek

108. Investigating chemoresistance mechanisms and collateral responses in pancreatic ductal adenocarcinoma [Poster Board #108]. **C. D'Inzeo**, V.D. Moore

109. Characterization of poly(aspartic acid) hydrolases from *pedobacter*, *erythrobacter* and *brevifollis* [Poster Board #109]. **T. Ho**, M. Weiland

110. Understanding the effect of obscurin and the RhoA pathway on cellular architecture and dynamics [Poster Board #110]. **K.D. Shultz**, S. Ouder Kirk, K. Kubow, C.J. Miller, N.T. Wright

111. Uncovering GMPK structures to define its catalytic mechanism [Poster Board #111]. **D. Rutan**, M.C. dela Cerna

112. Optimizing the expression and purification of the C-terminal domain of human cardiac troponin C for future calcium and cadmium binding studies [Poster Board #112]. **R. Sengelmann**, R. Warfel, A.M. Spuches

113. High-throughput characterization of DNA aptamers for cocaine detection [Poster Board #113]. **R. Hill**, O. Alkhamis, j. canoura, Y. Xiao

114. Biophysical characterization of the binding of novel PRL3 inhibitors [Poster Board #114]. **G.M. Bennett**, M.C. dela Cerna

- 115.** Functional characterization and *in silico* analysis of the PTPN18 catalytic domain [Poster Board #115]. **N. Dillon**, T. Spencer, **M.C. dela Cerna**
- 116.** Chemical probe screening for modulators of DUSP13 phosphatase activity [Poster Board #116]. **J. Rodriguez**, M.C. dela Cerna
- 117.** Recombinant expression of the kinase domain of atypical MAPK4 [Poster Board #117]. **J. Rodriguez**, M.C. dela Cerna
- 118.** Designers engineer functional proteins, we break them apart to see how they work [Poster Board #118]. **T. Spencer**, M.C. dela Cerna
- 119.** GenX and other PFAS pollution on plants in the Cape Fear River Basin [Poster Board #119]. **A.K. Locke**, S. Han
- 120.** Quantifying microplastic distribution in North Georgia creeks [Poster Board #120]. **K. Gray**, **A. Cabrera**, **A. York**, **a. dickson**, **T. Colson**, E. Crisp
- 121.** Microplastics investigations in water column and sediment of various streams in the Coosa watershed of northwest Georgia [Poster Board #121]. **K. Gray**, **A. York**, **T. Colson**, **A. Dickson**, **A. Cabrera**, R.E. Crisp
- 122.** Effect of the etching method on the specific surface area and pore size distribution of Ti_2Ct_x and $Ti_3C_2t_x$ MXenes for carbon dioxide capture applications [Poster Board #122]. **D.R. Bonilla**, O. Udoh, B.R. Gautam, D.E. Autrey
- 123.** Preparation, characterization, and reactivity of cationic, octahedral ruthenium (II) complexes supported by a single 4,4'-tert-butyl-2,2'-bipyridine ligand [Poster Board #123]. **A.R. Marks**, **K.G. Musso**, P.H. Ouedraogo, B.P. Quillian
- 124.** Optimization and characterization of wet-spinning biopolymer cellulose nanocrystals composite fibers [Poster Board #124]. **C. Cox**, O. Dickinson, T.A. Nile, A.G. Glenn, H. Leese
- 125.** Detection of nitroaromatic compounds using porphyrin-doped silica sol-gels [Poster Board #125]. **N. Snyder**, **S. Meere**, C.H. Lisse
- 126.** Wet spinning of fibers from cellulose dissolved in 1-Butyl-3-Methylimidazolium chloride (BMImCl) [Poster Board #126]. **B.G. Robinson**, **J.A. Scutari**, **S. Zhu**, **E. McDowell**, J.R. Alston
- 127.** Modifying the functional group on self-assembled monolayers to luminesce [Poster Board #127]. **F.I. Alam**, **R. Barnes**, C. Gray, **S.O. Sohaib**, **A. Kang**
- 128.** Isolation and investigation of a key intermediate in ruthenium photoredox catalysis [Poster Board #128]. **N. Dabney**, S.J. Horsewill, D.J. Scott, T.A. Nile, A.G. Glenn

- 129.** Synthesis of a colorimetric silica sol-gel sensor for the detection of methamphetamine [Poster Board #129]. **R.A. Jenkins**, C.H. Lisse
- 130.** Synthesis and structural analysis of complexes containing the bridging oxo, dicarboxylato diiron(III) core [Poster Board #130]. **G. Roberts**, C.W. Padgett, B.P. Quillian, W.E. Lynch
- 131.** Controlling drug release properties of tetraethyl orthosilicate (TEOS)-based sol-gel nanoparticles [Poster Board #131]. **R. Glover**, C.H. Lisse
- 132.** Copper-catalyzed reductive coupling of 2-Azatrienes and electrophiles for the synthesis of enantioenriched amines [Poster Board #132]. **A. Zhang**, P. Zhou, J. Zhu
- 133.** Polymerization of Lichen-Derived (+)-Usnic Acid [Poster Board #133]. **R.R. Zhou**, B. El-Zaatari
- 134.** Methodological investigation into the phosphorus extrusion of bipyridine [Poster Board #134]. **A. Dancer**, B. Wicker
- 135.** Electrocatalytic 1,3-difunctionalization of cyclopropanes for the construction of heterocycle [Poster Board #135]. **J. Zhang**, A. Nguyen, Q. Wang
- 136.** Efforts towards total synthesis of novel anti-austerity agents against PANC-1 human pancreatic cancer cell line [Poster Board #136]. **E. Wang**, Y. Zhao, I. Shin, H. Kim, J. Hong
- 137.** Fast, thiol-mediated, dynamic siloxane exchanges? [Poster Board #137]. **P. Bombard**, B. El-Zaatari
- 138.** Combating new modes of antibiotic resistance: Preparation of thiol-containing benzoxazoles for metallo- β -lactamase inhibition [Poster Board #138]. **S.A. Kuhn**, A.M. Duda, K.J. Franz
- 139.** Covalent incorporation of (+)-usnic acid into PDMS and peg polymer networks [Poster Board #139]. **J. Vargo**, B. El-Zaatari
- 140.** Separation and analysis of caffeine, theobromine, and theophylline in different coffee and tea samples via subcritical water chromatography [Poster Board #140]. **M. Hindi**, Y. Yang
- 141.** Designing and synthesizing potential drug candidates for viral infections [Poster Board #141]. **K.V. Truong**, J. Moore, S.S. Panda
- 142.** Design and synthesis of curcumin mimic hybrid conjugates as potential therapeutics for breast cancer [Poster Board #142]. **H. Dinkins**, D. Hansen, M. Thangaraju, B.L. Lokeshwar, S.S. Panda
- 143.** Impact of fluorination of polymer on charge photogeneration [Poster Board #143]. **J. Evans**, J. Hou, S. Han, **B. Gautam**

- 144.** Impact of fullerene derivative acceptor on morphology and charge delocalization in polymer blends [Poster Board #144]. D. Darden, S. Han, W. You, **B. Gautam**
- 145.** Exploring the molecular interactions driving cyclotide self-aggregation using molecular docking [Poster Board #145]. S. Nuh, C. Forlemu, B. Shepard, S. Mwongela, **N.Y. Forlemu**
- 146.** Molecular modeling of cyclotide self-aggregation and affinity with prolyl oligopeptidase [Poster Board #146]. Z. Adu, R. Aceves Mundo, C. Forlemu, B. Shepard, S. Mwongela, **N.Y. Forlemu**
- 147.** Towards a virtual pipeline for identifying PTP inhibitors [Poster Board #147]. **A. Brinegar**, M.C. dela Cerna
- 148.** Analyzing the equilibrium thermodynamics of amide-linked rhodamine B [Poster Board #148]. **A. Young**, R. Spera, B. Stratton, A. Pierre, P. Lundin, K.H. Fogarty
- 149.** Investigating the responses to light perturbations of the photosensitive Belousov-Zhabotinsky reaction [Poster Board #149]. **N. Whittle**, S. Nkomo
- 150.** Steric effects of *meso* and flanking dipyrin substituents on luminescence [Poster Board #150]. **L. Boyle**, **A. Chang**, **H. Kessler**, W. Dougherty, K. Hoffman, A.B. Scharf
- 151.** Comparing the impact of using different levels of Density Functional Theory (DFT) on a model for predicting toxicity [Poster Board #151]. **C. Takahashi**, S. Nkomo
- 152.** We asked AlphaFold2 to read SNIETORP just to see what happens [Poster Board #152]. **D. Rutan**, **T. Spencer**, M.C. dela Cerna
- 153.** Will ChatGPT succeed as our biochemistry lab manager? [Poster Board #153]. **G.M. Bennett**, A. Brinegar, M.C. dela Cerna
- 154.** Design of a series of laboratory experiences for general chemistry chemistry students on the quantitative and semi-quantitative analysis of reducing sugars in South Florida Honeys [Poster Board #154]. **A. Guerra**, **S. Serrano**, **G. Simon**, A.J. Rodriguez
- 155.** NO_x removal efficiency and washing resistance of iron oxide decorated g-C₃N₄ nanosheets attached to recycled asphalt pavement aggregate [Poster Board #155]. **E. Rose**
- 156.** Design, facile synthesis, and evaluation of a chalcone-based small molecule ULK1 agonist for the treatment of Huntington's Disease [Poster Board #156]. **C. McFadyen**, M. Bruno
- 157.** Eco-friendly design and fabrication of a microalgae-based sponge to efficiently remove oil from water for environmental remediation [Poster Board #157]. **D. Agarwal**, M. Bruno
- 158.** Design and synthesis of a novel small molecule interleukin-6 inhibitor for the amelioration of inflammatory bowel disease [Poster Board #158]. **S. Maruvada**, M. Bruno

159. Design and green synthesis of a novel imine resveratrol analog as a multi-target directed ligand for the treatment of Alzheimer's Disease [Poster Board #159]. **K. Jin**, M. Bruno

160. Purification and characterization of phyto-ceramides for the treatment of psoriatic epidermal damage [Poster Board #160]. **V. Villa**, M. Bruno

161. Rational design and synthesis of a PHD2 inhibitor for oral treatment of chronic kidney disease-induced anemia [Poster Board #161]. **C. Zhao**, T. Anglin

162. Transferrin-conjugated ionizable lipid nanoparticles for the delivery of mRNA across the blood-brain barrier [Poster Board #162]. **A. Mansoor**, M.J. Mitchell

163. Influence of methanol on aqueous solutions of coumarin 343 complexed with cucurbit[7]uril [Poster Board #163]. **P. Smitherman**, J. Cash, R. Spencer, M. Keeler, F.A. Khan, J.E. Hansen

164. Optimizing synthesis of gold and silver nanoparticles for paper-based electrochemical device fabrication [Poster Board #164]. **J. Perry**, C. Farling, Y. Xiao

Durham Convention Center
Junior Ballroom A3

Advances In Metal Catalysis for Organic Synthesis

Cosponsored by CATL and ORGN
Q. Wang, *Organizer*

11:00 Introductory Remarks.

11:05. New methods in regiodivergent transition metal-catalyzed hydro- and difunctionalization of dienes. **S. Malcolmson**, P. Zhou, X. Ma, A. Zhang

11:25. Solutions to challenges in aryne chemistry. **C. Roberts**

11:45. Recent advancement in gold redox chemistry: New transformations and asymmetric catalysis. **X. Shi**

FRIDAY AFTERNOON

Durham Convention Center
Junior Ballroom A2

Southeastern Magnetic Resonance Conference (SEMRC)

Cosponsored by ANYL and PHYS

A. I. Smirnov, M. A. Ter Horst, *Organizers*

12:45 Introductory Remarks.

12:50. Expanding hyperpolarization target scope and efficiency with new approaches to spin polarization transfer. **J. Lindale**, L. Smith, L. Everhart, M. Mammen, R.S. Raman, S. Eriksson, X. Li, W.S. Warren

1:05. Eliminating quadrupolar degradation of sabre hyperpolarization. **L. Smith**, J. Lindale, W.S. Warren

1:20. Decorrelated singlet and triplet exciton delocalization in acetylene-bridged Zn-porphyrin dimers. **M.Y. Teferi**, H. Medagedara, K. Mardis, A. Rury, J. Niklas, O. Poluektov

1:35 Break.

1:45. Engineering quantum coherence and control in diluted spin systems. **I. Chiorescu**, S. Bertaina, J. Cochran, G. Franco

2:00. Magnetic resonance and optical studies of high pressure high temperature synthesized diamond microparticles with controlled nitrogen content. **N. Nunn**, S. Milikisiyants, M. Torelli, A. Healey, R. Styles, B. Johnson, P. Reineck, C. Long, T. Dumm, A. Dalis, T. Oshima, E. Druga, A. Ajoy, A.I. Smirnov, O. Shenderova

2:15. Massive hyperfine interactions in Ln^{II} complexes. **J. Hruby**, K. Kundu, D. Ngo, H. Kwon, Z. Ma, T. Harris, P. Smith, S. Minasian, R. McClain, B.G. Harvey, J.R. Long, S. Hill

2:30. Quantum sensing by nanodiamond via magnetically-induced fluorescence contrast. **M.D. Torelli**, N. Nunn, M. Voynov, A.I. Smirnov, O. Shenderova

Durham Convention Center

Grand Ballroom I

Undergraduate Poster Session

Cosponsored by CHED

J. A. Feducia, K. C. Glasgow, *Organizers*

12:50 - 2:50

- 101.** Effect of the mobile phase in the retention times of antiarrhythmic drugs in high performance liquid chromatography [Poster Board #101]. **A.S. Fordham**, L. De La Garza
- 102.** Analysis of heavy metals in comparable organic and non-organic food and beverage products by atomic absorption spectroscopy (AAS) [Poster Board #102]. **V. Martin**, S.E. Hooper Marosek
- 103.** Analysis of phenolic compounds found in beer as a function of malt terroir using HPLC and HR-LCMS [Poster Board #103]. **A. Wujick**, C. Balog, C. Paoletta, D. Liskin, A. Higgs, K. Kingsbury, A. Brehm, A. Brockway, R.A. Quinlan
- 104.** The metal binding properties of a 2-aminophenanthroline substituted coumarine imine ligand [Poster Board #104]. **E. Sower**, Y. Yuan, K.J. Wallace, M. Bonizzoni
- 105.** Colorimetric characterization of ligands for metal cation detection [Poster Board #105]. **B. Meredith**, T. Kesharwani, **P.P. Benz**
- 106.** 3D-printed visible light spectrometer [Poster Board #106]. **H. Braden**, T. Cosby
- 107.** Investigating the effect of divalent metal ions on the activity of GAPDH derived from *Escherichia coli* [Poster Board #107]. **S. Repala**, T. Outlaw, A. Robison, I. Williams, K.J. Franz
- 108.** Comparative study of visible and radio spectroscopy for identifying chemical compounds on meteors [Poster Board #108]. **J. Freeman**, M. Leake
- 109.** Analysis of amoxicillin/clavulanic acid tablets from low-and-middle income countries by high performance liquid chromatography [Poster Board #109]. **A. Myers**, M.E. Turner
- 110.** Amplification-by-polymerization in protein biosensing [Poster Board #110]. **K. Williams-McCord**, P. He
- 111.** Detection of antimicrobial properties of several herbal and fruit teas via a choline kinase inhibition assay [Poster Board #111]. **A. Brock**, S. Ibrahim, T. Zimmerman
- 112.** Novel expression and characterization of lactate monooxygenase from *Thermus thermophilus* [Poster Board #112]. **A. Nimmo**, M. Wiseman, K. Kean
- 113.** Novel expression and characterization of lactate monooxygenase from *Halopiger salifodinae* [Poster Board #113]. **M. Wiseman**, A. Nimmo, K. Kean
- 114.** Loratadine influence on MRSA ATP levels [Poster Board #114]. **G. Valenzano**, H.B. Miller, M.S. Blackledge
- 115.** Optimizing a *C. elegans* infection model to evaluate antibiotic adjuvants against MRSA [Poster Board #115]. **C. Cox**, H.B. Miller, M.S. Blackledge

- 116.** Loratadine, the antihistamine, modulates hemolysin gene expression in MRSA [Poster Board #116]. **H. Balogh**, B. Viering, V. Federico, G. Valenzano, M.S. Blackledge, H.B. Miller
- 117.** Loratadine impacts the formation of persisters in MRSA [Poster Board #117]. **T. Federico**, B. Viering, M.S. Blackledge, H.B. Miller
- 118.** Expression, purification, and characterization of carbonic anhydrase from *Deiniococcus radiodurans* [Poster Board #118]. **P. Nyboer**, N. Khan, K.M. Kean
- 119.** Investigating pH sensitivity of rhodamine B amide derivatives [Poster Board #119]. **R.J. Spera**, B. Sobolewski, A. Pierre, P. Lundin, K. Fogarty
- 120.** Modeling glutathionylation by installing a redox-inert bioisostere [Poster Board #120]. **G. Laws, J. Morgan, E. Peterson**, T. Zaman
- 121.** Expression, purification, and characterization of a novel carbonic anhydrase from *Hypsibius exemplaris* [Poster Board #121]. **N. Khan**, P. Nyboer, K.M. Kean
- 122.** 4-Phenylbutyrate promotes mitochondrial biogenesis and metabolism in C2C12 myotubes while increasing extracellular BCAA concentrations during insulin resistance [Poster Board #122]. **T. Zaman, R. Watne**, C. Rivera, C. Smith, R. Vaughan, A.J. Wommack
- 123.** Investigation of tetrahydrocannabinol (THC) analogues in North Carolina [Poster Board #123]. C. Taylor, P. Vanada, **J. Thorpe**
- 124.** Assessing the health of the Little River: Stream sampling and *Escherichia coli* monitoring [Poster Board #124]. **I. Wright**, N. Duncan
- 125.** The ligand exchange of iron oxide nanoparticles and peptoids for the Advancement of MRI technology [Poster Board #125]. **G. Johnson**, K. Cavey, M. Zhang, P.G. Van Patten
- 126.** Synthesis and spectroscopic characterization of phenothiazine ionic liquids [Poster Board #126]. **W. Collier**, O.A. Cojocar
- 127.** Can chromium(III)-DNA-small molecule ternary complexes be formed? [Poster Board #127]. S. Marchi, **G. Sunde, E. Wilkes, K. Kovitch**, S.A. Woski, J.B. Vincent
- 128.** Towards liquid state trihexyphenidyl drugs for the treatment of Parkinson's disease [Poster Board #128]. **D. Popa**, O.A. Cojocar
- 129.** Biomimetic design of mechanochromic single chain nanoparticle polymer networks [Poster Board #129]. **S. Robinson**, M.H. Barbee
- 130.** Synthesis and characterization of ruthenium (II) polypyridyl silatranes as carbon dioxide reduction catalysts [Poster Board #130]. **B. Butler**, S.J. Tereniak, G.J. Meyer

- 131.** Synthesizing single chain polymer nanoparticle networks [Poster Board #131]. **K. Hooper**, M.H. Barbee
- 132.** Synthesizing single chain polymer nanoparticle networks by reinitiating raft [Poster Board #132]. **D. Donovan**, M.H. Barbee
- 133.** Quantifying lateral interactions in gold self-assembled monolayers: The effect of topography and surface concentration [Poster Board #133]. **A.X. Vu**, T.S. Teitsworth, M.R. Lockett
- 134.** Using multi-step synthesis for the production of hydrogels with adhesive properties [Poster Board #134]. **C. Smith**, C.H. Lisse
- 135.** Preparation of Chromenoquinoxaline derivative: New leads for treating er+ cancers [Poster Board #135]. **R. Artis**, K. Nguyen, B.P. Quillian
- 136.** *N*-acyl hydrazone furfural derivatives as novel tools for disrupting microbial biofilm formation [Poster Board #136]. **I. Abdullaeva**, D. Ferguson, K. Murphy
- 137.** Towards liquid state trifluoperazine drugs [Poster Board #137]. **S. Beshara**, O.A. Cojocar
- 138.** *N*-acyl hydrazone and semicarbazide furfural derivatives as novel tools for disrupting microbial biofilm formation [Poster Board #138]. **D.K. Ferguson**, K. Murphy
- 139.** Synthesis of sigma 2 receptor ligands as potential analgesics [Poster Board #139]. **B.C. Brusseau**, P.S. Dhote, S. Haider, N.V. Nucci, T.M. Keck, K.J. Frankowski
- 140.** The development of *N,N*-*trans*-spanning ligands [Poster Board #140]. **B.C. Higgs**, L. Hair, M. Akama, M. James, C. McMillen, J.A. Pienkos
- 141.** Initial characterization of two putative poly(aspartic acid) hydrolases from *Sphingopyxis* and *Sphingomonadales* [Poster Board #141]. **W. Callaway**, M. Weiland
- 142.** Synthesis of fluorene-based macrocycles for untangling of polystyrene-based nanoplastics [Poster Board #142]. **W. Gibson**, K. Murphy
- 143.** Alkynyl iodide-based halogen-bonding with isocyanides to improve utility [Poster Board #143]. **N. Antoine**, M. James, K. Dungey, J.A. Pienkos
- 144.** Exploration of a new intermolecular photo-dehydro-Diels-Alder reaction [Poster Board #144]. **E. Eakins**, W. Yang
- 145.** Alternative green synthesis of the pesticide carbaryl [Poster Board #145]. **C. Underwood**, **T. Walters**, **R. Okoth**

- 146.** Efforts towards the synthesis and biological evaluation of artocarpesin and structural analogs [Poster Board #146]. C. Edwards, **K. Soma**, J.G. Pierce
- 147.** Physicochemical properties of trifluoroacetamido derivatives of acetaminophen and acedoben [Poster Board #147]. **J.A. Boldon**, T.A. Shell
- 148.** Developing a method for high-energy pulsed laser ablation in anhydrous liquids under inert gas [Poster Board #148]. **S. Calhoun**, O. Nachtigall
- 149.** Photocatalyzed hyperpolarization of nitrate using signal amplification by reversible exchange [Poster Board #149]. **E.L. Messina**, E. Brown, F.N. Castellano
- 150.** Observing refractive changes in fluids through use of a schlieren system outdoors [Poster Board #150]. **A. Boers**, H. Park
- 151.** Theoretical studies of hydrogen abstraction from fluorinated acetone and fluorinated acetaldehyde [Poster Board #151]. **L.E. Washburn**, T.V. Albu
- 152.** Simulating exciton dynamics and spectra in organic semiconductor thin-films [Poster Board #152]. **P. Tolley**, A. Olagbemi, J.J. Foley
- 153.** Characterization of free radical species generated by nano-additives in petroleum-based lubricants [Poster Board #153]. **P. Bankaitis**, R. Rana, J. Matheny, T. Smirnova
- 154.** Adsorption isotherm and kinetic studies of sodium fluorescein removal in aqueous solution by ZNR [Poster Board #154]. **D. Desai**, M. Caver, R. Dosi, J.C. Poler
- 155.** Synthesizing a conductive PEDOT/alginate hydrogel to match the physical and electrical properties of myocardial tissue [Poster Board #155]. **G. McNamara**, T. Anglin
- 156.** Improving lead sequestration and power conversion efficiency in organic-inorganic lead halide perovskite solar cells through external *alginate-L-cysteine* biopolymer encapsulation [Poster Board #156]. **A. Meduri**, M. Bruno
- 157.** Chemical recycling of poly(lactic acid) using a 1,1,3,3-tetramethylguanidinium zinc chloride catalyst [Poster Board #157]. **H. Manchi**, T. Anglin
- 158.** Nanomaterials-based electrochemical amyloid β immunosensors for early diagnosis of Alzheimer's disease [Poster Board #158]. **A. Garcia**, B. Core, D.E. Autrey, B.R. Gautam, Z. Luo, S. Han
- 159.** Investigating serotonin dynamics and simulating effects of antidepressants using variation in enzyme expression [Poster Board #159]. **A.J. Diefes**
- 160.** Micellar delivery of the immunotherapeutic 15-deoxy-D^{12,14}-prostamide J₂ for treatment of colon cancer [Poster Board #160]. **E. Fisher**, T. King, T. Hales, R. Van Dross, C. Burns

161. Factors limiting the formation of Fe-S clusters for nitrogen fixation by the NifUS system [Poster Board #161]. **N.M. Woodlief**

162. Random numbers and their applications [Poster Board #162]. **M. Dixon**, X. Tao

163. Characterizing the effect of VASP-profilin interaction on actin assembly [Poster Board #163]. **K. Wang**, N. Mann, R. Hughes

164. Creating a molecular bandaid for ACM [Poster Board #164]. **M. Benes**

165. Insights into the extension past 8-oxo-2'-deoxyguanosine with two Y-family polymerases [Poster Board #165]. **W. Ko**, M. Hamm

Durham Convention Center
Junior Ballroom D1

#SciComm: Advancing Inclusive Public Engagement with Science Using Various Communication Tools

Cosponsored by CPT
N. Neal-Walthall, I. Walker Karega , *Organizers*

1:00 Introductory Remarks.

1:05. Using participatory science to identify and communicate chemical water quality risks in Guatemala City tap water. **J. Hoponick Redmon**

1:20. Public radio for inclusive storytelling about science: The measure of everyday life as a model. **B. Southwell**, M. Gentry

1:35. Integrating comedy writing into science communication. **B. Ma**

1:50. Development of chemistry classroom and laboratory learning modules for blind and visually impaired high school and undergraduate students. **R. Dabke**, S. Melaku, J. Schreck, G. Kameron, M. Harrell, L. Ray, H. Turner

Durham Convention Center
Junior Ballroom A1

Advances in Mass Spectrometry: Contributions from Students

Cosponsored by ANYL
A. L. Patrick, *Organizer*

1:00 Introductory Remarks.

1:05. Noncovalent mononuclear copper complexation for high-throughput chiral drug differentiation using ion mobility-mass spectrometry. **B. Blakley**, E. Zlibut, J.C. May, J.A. McLean

1:20. Targeting flavor: Integration of GC/MS and LC/MS data in targeted and untargeted metabolomic workflows to reveal molecular transformations throughout brewing and fermentation of a SMaSH beer. **A.V. Lo Presti**, A.R. Cicali, L. Marsh, A.E. Outhous, L.R. Weber, S. Harper, S.A. Morton, C.A. Hughey

1:35. Enhanced separation of synthetic cannabinoid metabolite isomers using slim high-resolution ion mobility-mass spectrometry (HRIM). **R. Aderorho**, C.D. Chouinard

1:50 Intermission.

2:00. Liquid chromatography - Ion mobility - tandem mass spectrometry for discrimination between pathogenic and non-pathogenic E. coli strains using the metabolome, lipidome and proteome. **O.E. OLAJIDE**, K.Y. Kartowikromo, Y. Yi, J. Zheng, A.M. Hamid

2:15. Mass spectrometry technique for detection of polyfluorinated substances. **E. Hayden**, J.C. Poler

2:30. Real-time quantification of gas-phase PFAS with iodide chemical ionization mass spectrometry via external calibration with liquid standards. **M. Davern**, G.V. West, J. Surratt, B.J. Turpin, Y. Zhang

Durham Arts Council
IBM Rehearsal Hall

Biochemistry Research and Development

D. A. Canelas, *Organizer*

1:00 Introductory Remarks.

1:05. Conical intersection accessibility dictates brightness in red fluorescent proteins. **E. Pieri**, A. Walker, M. Zhu, T.J. Martinez

1:20. Recombinant expression of NnIA homologs shows widespread *N*-Nitroglycine degradation activity amongst bacteria. **K.A. Strickland** , **B. Martinez Rodriguez**, A.A. Holland, H. Silverio, S. Wagner, M. Luna-Alva, J.D. Caranto

1:35. Enhancing the combinatorial biosynthesis of polyketides via acyltransferase engineering. **S. Welch**, G.J. Williams

1:50 Intermission.

2:00. Characterization of polyamidoamine dendrimers as delivery carriers for nucleic acid nanoparticles. **B. Rawlins**, Y. Avila , L. Rebolledo, E. Skelly, K. Afonin

2:15. Circumventing roadblocks in NADPH oxidase inhibition. **A. Develin**, J.D. Sieber, B. Fuglestad

2:30. Characterization of phospholamban phosphorylation in response to β 1-adrenoceptor stimulation in cardiac H9c2 myocytes. **N.U. Anyiam**

Durham Arts Council
PSI Theatre

Inorganic Chemistry Research and Development

Cosponsored by INOR
D. A. Canelas, J. M. Harrington, *Organizers*
K. Haas, *Presiding*

1:00 Introductory Remarks.

1:05. Chaperoning copper in extracellular spaces. **K.L. Haas**

1:20. Structural isomers of quinoline-derived meridional ligands in homoleptic cobalt complexes. **D.P. Harrison**, A. Hernandez, J. Stober, J. Dickenson

1:35. Frustrated magnetism of mixed-metal fluoride pyrochlores $A_xM^{\text{II}}_xM^{\text{III}}_{(2-x)}F_6$. **L. Weragoda Masachchi**, H. zur Loye

1:50 Intermission.

2:00. Carbon monoxide activation with Re(III) complexes. **L. Gouveia**, A.K. Adegboyega, E.A. Ison

2:15. Determining factors required to favor concerted proton-coupled electron transfer in tungsten hydride complexes. **D. Isaacs**, J.L. Dempsey

2:30. Electrolytic reactive carbon capture by iron tetraphenylporphyrin. **J. Thomas**, J. Stanely, J.Y. Yang

2:45. Chromium tricarbonyl complexes for Arene activation in Pd catalyzed C-H functionalization. **D. Griffin**, T. Brewster

Durham Convention Center
Junior Ballroom C

Organic Chemistry Research and Development

Cosponsored by ORGN
D. A. Canelas, *Organizer*
K. J. Frankowski, *Presiding*

1:00 Introductory Remarks.

1:05. Electrochemical diversification of nitrogen heterocycles. **K.J. Frankowski**, F. Wang

1:20. Remarkable rate acceleration of the Kemp elimination of benzisothiazoles and benzisoxazoles in mixed solvents. **M. Forconi**

1:35. Design and synthesis of potential NQO1 inhibitors using a molecular hybridization approach. **S. Patel**, S.S. Panda

1:50 Break.

2:00. Bench stable pyryliums and xanthyliums for catalytic reductions. **W.A. Hearne**, M.R. Gagne

2:15. 3,6-Bis(acetyloxy)-9H-Xanthen-9-one synthesis via annulation and acetylation. R.E. Lee, **H. Woo**, P.E. Heiple, J.C. O'Dell, V.L. Whitlock

Durham Convention Center
Junior Ballroom D2

Polymer Chemistry and Materials Science Research and Development

Cosponsored by PMSE and POLY
D. A. Canelas, *Organizer*
F. Zhang, *Presiding*

1:00 Introductory Remarks.

1:05. Design and development of sugar-based polycarbonates for therapeutic delivery. **F. Zhang**

1:20. Photochemical 3D printing of bioresorbable microneedle arrays for controlled transdermal drug delivery. **A. Bahnick**, A. Chou, Z. Leng, E.K. Augustine, M.I. Segal, M. Becker

1:35. Use of silane self-assembled monolayers to inhibit methicillin-resistant *Staphylococcus aureus* biofilm formation. **E. Gillis**, P. Lundin, M.S. Blackledge, B. Fiser

1:50 Break.

2:00. Characterization of sequence-dependent conformation of a disordered peptoid library. **E. Day**, S. Chittari, A. Knight

2:15. Synthesis of polymer-nucleobase composites for chemotherapy drug capture. **G. Su**, M.D. Schulz

2:30. Chitosan-*k*-carrageenan molecularly imprinted polymers (MIPs) for sequestration of bupivacaine. **J. Macasinag**

Durham Convention Center
Junior Ballroom D3

SERMACS: Hosting, Planning, Best Practices and More

Cosponsored by LAB
B. D. Feske, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05. Introduction to SERMACS, Inc.. **B.D. Feske**

1:25. Chris Bannochie - General Chair of SERMACS 2006 and 2018. **C.J. Bannochie**, T. Whiteside

1:45 Intermission.

1:55. Tracy Hamilton - General Chair of SERMACS 2021. **T.P. Hamilton**

2:15. Will Lynch - General Chair of SERMACS 2019. **W.E. Lynch**

2:35 Roundtable with SERMACS Executive Committee.

Durham Arts Council
Duke Rehearsal Hall

Single-molecule Dynamics in Complex Chemical and Biological Systems

Cosponsored by PHYS
A. Gahlmann, K. Welsher, *Organizers*

1:00 Introductory Remarks.

1:05. Structural dynamics during telomere loop formation studied by smFRET *in vitro*. **H. Lee**,
A. Lacen

1:25. ABEL-PIE: Pulsed interleaved excitation in the ABEL trap to measure single-molecule
dynamics. **A. Squires**

1:45. Real-time 3D single-particle tracking in an electric field: From mobility to active control.
A. Johnson

2:00 Intermission.

2:10. Monitoring the phosphorylation cycles of single molecules in solution. **Q. Wang**

2:30. Multi-parameter super-resolution optical imaging of single nanoparticles. **K.A. Willets**

2:50 Concluding Remarks.

Durham Convention Center
Meeting Room 3

Structure-Based Drug Design

Cosponsored by MEDI and ORGN
R. J. Bienstock, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05. Development of KOR agonists for non-addictive pain relief. **A. Trojniak**, R. Russo, V.
Dang, L. Mather, K. Koehn, A. Ravichandran, M. Cameron, L. Bohn, J. Aube

1:20. Hijacking beta-lactamase activity: Prodrugs designed to selectively kill drug-resistant
bacteria. **A.M. Duda**, H.R. Ma, L. You, K.J. Franz

1:35. Utilization of Hauser annulations to obtain and derivatize antibiotic Thermorubin. **Z. Kohanov**, A.N. Lowell

1:50 Break.

2:00. Benzimidazoles as Spingosine-1-phosphate transporter SPNS2 inhibitors. **C. Shrader**, W.L. Santos

2:15. Improving potency and oral bioavailability of Spns2 inhibitors *via* tail modifications. **K. Dunnavant**, W.L. Santos

2:30. Plight of CORMs: A case study of when designs lack strong structural and molecular foundations. **N. Bauer**, X. Yang, Z. Yuan, B. Wang

2:45 Session Closing.

Durham Convention Center
Meeting Room 4

Trends, Challenges, and Opportunities in Chemical Laboratory Safety

Cosponsored by CHAS
M. B. Koza, S. Sigmann, *Organizers*

1:00 introduction.

1:05. Microcredentialing – New Frontier in undergraduate safety training. **M.C. Box**

1:20. Creation, assessment, and application of postgraduate virtual reality experiences in laboratory safety. **D.S. Lawrence**

1:35. Improving chemists' safety in research and development laboratories: By eliminating all bench-level obstructions with a MAC hood support safety device. **T.D. McKibben**

1:50 break.

2:00. Accessing chemical hazard and safety data via the internet. **A.J. Williams**, T. Martin, V. Tkachenko

2:15. Applying lessons of NOD to chemical laboratory safety. **R.H. Hill**

2:30. Understanding, developing, and implementing laboratory safety culture in academic institutions. **D.F. Henry**

Durham Arts Council
Adaron Hall

Ultrafast and Nonlinear Spectroscopy

E. Ghadiri, L. Wang, *Organizers*
A. Salam, *Presiding*

1:00 Introductory Remarks.

1:05. Functional energy materials: From fundamental photophysics to device applications. **L. Wang**

1:25. Sensing polaron environment in a conducting polymer via the photoinduced Stark effect. **C. Grieco, A. Umar, A.L. Dorris**

1:45 Intermission.

1:55. Molecular QED: Basic theory, elementary applications, and some recent studies. **A. Salam**

2:15. Interfacial electron transfer in Fe(II)-polypyridine-TiO₂ assemblies: A computational perspective. **E. Jakubikova**

2:35. Wave function delocalization and ultrafast transport in optical microcavities. **R.F. Ribeiro**

Durham Convention Center
Junior Ballroom A3

Advances In Metal Catalysis for Organic Synthesis

Cosponsored by CATL and ORGN
Q. Wang, *Organizer*

1:30 Introductory Remarks.

1:35. Development of a nickel-catalyzed process for the manufacture of Belzutifan. **J. Hethcox**

1:55. 1,2-difunctionalization of 1,3-dienes through metal and metal-free methods. **B. Hemric, S. Baldassarre, A. Barni, A. Louise**

2:15. Enantioselective C-C bond formation via organoboron compounds. **M. Chen**

FRIDAY EVENING

Durham Convention Center
Grand Ballroom I

Southeastern Magnetic Resonance Conference (SEMRC)

Cosponsored by ANYL and PHYS
A. I. Smirnov, M. A. Ter Horst, *Organizers*

5:00 - 7:00

- 101.** Designing low-cost resistive coils for improving field homogeneity in single-sided NMR systems [Poster Board #101]. **S. Li, S. Rubin,** E. Van Valkenburgh, T.K. Meldrum
- 102.** Structural consequences of introducing bioactive domains to designer β -sheet peptide self-assemblies [Poster Board #102]. **A. Robang,** A.K. Paravastu
- 103.** Machine learning in nanoscience: A framework to enhance the efficacy of magnetic nanoparticle-based drug delivery in cancer patients [Poster Board #103]. **F.A. Adrah,** I. Yawlui, D. LaJeunesse
- 104.** Assignment of the dog allergen Can f 1 for antibody epitope mapping [Poster Board #104]. **E.F. Derose,** S.A. Gabel, J. Min, L.C. Pedersen, G. Mueller
- 105.** Structure elucidation of novel cyanobactins isolated from a cultured cyanobacterial strain of *Microcystis aeruginosa* [Poster Board #105]. **C. Agee,** W.K. Strangman, M.J. Recchia, R.T. Williamson
- 106.** Effect of metal ions on the chemical shift and relaxation time of acetate ions in aqueous solution [Poster Board #106]. **P. Randolph,** T.C. Devore
- 107.** Photoinduced electron spin polarization of platinum(II) complexes possessing one- and two Nitronyl-nitroxide radicals [Poster Board #107]. **A.M. Nogueira,** A. MARRI, D.A. Shultz
- 108.** Investigating structural and dynamic rearrangements in the functional regulation of a classically allosteric protein [Poster Board #108]. **D.J. Vera-Rodriguez,** P.J. Sapienza, A. Lee
- 109.** High temperature annealing studies of fluorescent diamond particles hosting nitrogen vacancy centers [Poster Board #109]. **N. Nunn,** S. Milikisiyants, M. Torelli, A.I. Smirnov, O. Shenderova
- 110.** Multipronged approach to profiling metabolites in *beta vulgaris* L dried pulp extracts using chromatography, NMR, and other spectroscopy methods [Poster Board #110]. **J. Fiadorwu**

- 111.** Assessing local pH in sterically-restricted environment from changes in rotational motion of EPR probes [Poster Board #111]. **M.A. Voinov**, A.I. Smirnov, T.I. Smirnova
- 112.** Hyperpolarization of imidazole in pure D₂O via signal amplification by reversible exchange (sabre) for MRI pH sensing [Poster Board #112]. **M. Abdulmojeed**, S. McBride, A. Davidsson, K. Macculloch, A. Browning, T. Theis
- 113.** Zero- to ultra-low field NMR: Quantifying SABRE hyperpolarization with a Rb vapor cell magnetometer [Poster Board #113]. **A. Ortmeier**, T. Theis
- 114.** Utilizing visible light photosensitization for *para*-hydrogen induced hyperpolarization [Poster Board #114]. **E. Brown**, I. Mandzhieva, P.M. TomHon, T. Theis, F.N. Castellano
- 115.** Hunting evidence of aggregation in ADP and the influence of ion binding [Poster Board #115]. **K. Marr**, A. Jerschow
- 116.** Determining effectiveness of a catalyst on the depolymerization of polyethylene terephthalate using kinetics [Poster Board #116]. **Z. Jackson**, D. Savage, M. Davidson, T.A. Nile, A.G. Glenn
- 117.** Distance dependence of photoinduced electron spin polarization of exchange-coupled biradicals [Poster Board #117]. **A. MARRI**, D.A. Shultz
- 118.** Electron spin resonance spectroscopic study of thymol and carvacrol radicals [Poster Board #118]. **H.J. Sipe**
- 119.** Solid-state NMR structural studies of thermochromic peptide-polymer hybrid systems [Poster Board #119]. **T. Rao Sudarshan**, A.K. Paravastu
- 120.** Site-directed spin labeling of oxalate decarboxylase from *Bacillus subtilis* [Poster Board #120]. **U. Athar**
- 121.** Late stage assembly of para-aminobenzoate by the self-sacrificial enzyme CADD [Poster Board #121]. H.N. Phan, O.M. Manley, L. Cha, D. Hilovsky, W. Chang, **P. Thompson**, X. Liu, T.M. Makris
- 122.** ¹³C-enhanced ¹³C-¹³C and ¹³C-¹H correlations in liquid state NMR by utilizing e⁻-¹³C scalar-coupling Overhauser DNP [Poster Board #122]. **S. Wi**, t. dubroca, J. Van Tol, T. Orlando, L. Frydman, S. Hill
- 123.** Examination of exogenous and endogenous irradiation effects on PuO₂ and its precursors via EPR spectroscopy [Poster Board #123]. **J.S. Kinyon**, E. Villa-Aleman, B. Foley
- 124.** Visualizing a protonated RNA state in mGHG bulge motifs [Poster Board #124]. **J.A. Boyer**

- 125.** Leveraging the power of solid-state NMR to probe peptide-lipid interactions in membranes containing lysolipids that influence spontaneous curvature [Poster Board #125]. **A.C. Zourou**, R. Fu, E.P. Goodell, M. Cotten
- 126.** Investigating lipid phase behaviors in relation to direct membrane translocation by cationic peptides: A solid-state NMR study [Poster Board #126]. **E. Goodell**, R. Fu, M. Cotten
- 127.** SABRE dynamics of current generation PET tracers [Poster Board #127]. **B. Dhali**, M. Pike, K. Macculloch, A. Browning, T. Theis
- 128.** Fluorescent diamond particles for lateral flow assay [Poster Board #128]. **G. Eberle**, N. Nunn, M. Torelli, C. Marcinkiewicz, M. Sternberg, G. Maddock, M. Mansfield, J. Gerstenhaber, G. Feuerstein, O. Shenderova
- 129.** Multi-functional role of oxalate decarboxylase revealed by EPR studies [Poster Board #129]. **Z. Becerra**, A. Angerhofer
- 130.** Supramolecular delivery systems for carotenoids: EPR and optical studies [Poster Board #130]. **A.L. Focsan**, N. Polyakov, Y. Gao, L. Kispert
- 131.** Microfluidic-enabled microresonators for sub-microliter, sub-micromolar electron paramagnetic resonance spectroscopy of spin-labeled proteins [Poster Board #131]. N. Abhyankar, M. Catterton, G. Cooksey, **V.A. Szalai**
- 132.** Hydrogen bonding and nonpolar environment applications to some rare carotenoids [Poster Board #132]. **A.L. Focsan**, Y. Gao, N. Polyakov, L. Kispert
- 133.** Coherences of photo-induced electron spin qubit pair states in photosynthetic proteins [Poster Board #133]. **J. Bindra**, J. Niklas, L.M. Utschig-Johnson, O. Poluektov
- 134.** Gadolinium-based contrast agent (hproca32.collagen1) for magnetic resonance imaging of fibrotic diseases [Poster Board #134]. **F. Akinlotan**, O.S. Bamishaye, D. Li, Z. Gui, J. Qiao, M. Kirberger, J. Yang
- 135.** Freeze-drying to supercritical drying: Comparing the effect of drying method on the morphology of bacterial cellulose [Poster Board #135]. **R. Kulkarni**, J.R. Alston
- 136.** Enabling the early detection and staging of chronic diseases by collagen-targeted MRI protein contrast agent (hproca32.collagen1) [Poster Board #136]. **S.o. Bamishaye**, J. Qiao, J. Yang, Z. Gui, F. Akinlotan, D. Li, M. Kirberger
- 137.** Relaxometric studies of an unmodified and modified Octanuclear iron cluster for implications in MR imaging [Poster Board #137]. **R.A. Banner**, R.G. Raptis
- 138.** Computer optimization of multi-axial pulse shapes to generate hyperpolarization of ^{13}C -acetate within a SABRE regime [Poster Board #138]. **L. Everhart**

SATURDAY MORNING

Durham Convention Center
Grand Ballroom I

Undergraduate Poster Session

Cosponsored by CHED
J. A. Feducia, K. C. Glasgow, *Organizers*

8:30 - 10:30

139. Analysis and comparison of commercial glow sticks [Poster Board #139]. G.H. Lowke, **C.E. Dahm**

140. Birdcage coil testing for 21t pre-clinical imaging [Poster Board #140]. **T. Vanderlinden**, M. Elumalai, S. Grant

141. Microgreens: Does a micro or macro change occur when grown in Earth, lunar, and Martian simulant soils? [Poster Board #141]. **M.M. Brown**, J.R. Willis, S. Varnum, K.W. Barnes

142. Investigation into the purity of various essential oils via GC-MS [Poster Board #142]. C. Chirombe, **S. West**

143. Macrocyclic amine synthesis – in search of improved methods [Poster Board #143]. **D.J. Savoie**, A. Lajmi

144. Chemometric analysis of absorbance and fluorescence data from South Florida honeys [Poster Board #144]. **L. Harrison, M. Shelley**, A.J. Rodriguez

145. Hit me with your best shot: A comparative analysis in Starbucks' coffee grounds and espresso quality [Poster Board #145]. **J.R. Willis**, M.M. Brown, S. Varnum, D. Scheffler, K.W. Barnes

146. Understanding how NtrZ affects NtrY in *Caulobacter crescentus* [Poster Board #146]. **Z. Dominick**, B. Stein

147. Effect of NtrX phosphorylation on DNA binding in *Caulobacter crescentus* [Poster Board #147]. **R. Lanam**, B. Stein

148. Development of a covalent labeling assay of quorum sensing enzyme LuxS [Poster Board #148]. **S. Pruett**, E. Glass, C. McMahon

- 149.** Investigating the effects of TcdA and sulfur reductants on the formation of tRNA modification ct^6A [Poster Board #149]. **B. Michel**, M.A. Addo, J. Ribeiro Filho, P.C. Dos Santos
- 150.** Untargeted metabolomics approach for the screening of endometrial cancer [Poster Board #150]. **B. Garrison**, K. Amrhein, S. Richards, J. Troisi, M. Lombardi, S.J. Symes
- 151.** Targeted natural product discovery from marine parasite microbiomes [Poster Board #151]. **M. Swan**, S. Bennett, C. Agee, V. Gadikota, E. Smith, R.T. Williamson, W.K. Strangman
- 152.** Expression and characterization of bacterial lectin towards development of anti-adhesion molecules [Poster Board #152]. **Q. Nyberg**, C. McMahon
- 153.** Inhibition of autoinducer-2 quorum sensing pathway by targeting the LuxS enzyme [Poster Board #153]. **A. Coffey**, A. Blatz, C. McMahon
- 154.** Creation of guanidinium-based antibiotic-adjuvant hybrids to bypass the outer membranes of Gram-negative bacteria [Poster Board #154]. **K. Handy**, A.L. Wolfe
- 155.** Optimization of multivalent protein bioconjugates using non-canonical amino acids [Poster Board #155]. **R. Gourdie**, **E. Boyt**, D.D. Young
- 156.** Study of small molecule-induced CCG repeat contraction [Poster Board #156]. **E. Duck**, W. Yang
- 157.** Developing an inhibitor of XPA-RPA interaction using a fragment-based drug discovery approach [Poster Board #157]. **M.O. Pierce**, A. D'Souza, W.J. Chazin
- 158.** Catalyst Lasso length: How linker length effects the production of biofuel [Poster Board #158]. **G.D. Coulter**, T. Vasicek
- 159.** Assessing the use of Bobbitt's salt in the study of environmental oxidations [Poster Board #159]. **J.C. Burdette**, J.M. Bray, A.I. Goranov, K.M. Lambert
- 160.** Determination of water quality parameters by a colorimetric method at Isla Verde Marine Reserve [Poster Board #160]. **J. Alvarez Cagua**, **E. Rosario-Marrero**, L.I. Santiago Perez, N. Ortega Reyes
- 161.** Identification of microplastics in South Florida honey [Poster Board #161]. **C. Ibarra**, A.J. Rodriguez
- 162.** Synthesis of biomolecule-AuNPs for potential use as temperature sensitive biomarkers [Poster Board #162]. **K. Merritt**, **B. Hawk**, G.A. Giles
- 163.** Desorption of immobilized catalysts: Comparison of two immobilization methods [Poster Board #163]. **S. Fink**, T. Vasicek

- 164.** Functionalized gold nanoparticles as molecular probes: Harnessing the potential of halogen-bonding in detection schemes [Poster Board #164]. **K. Lalwani**, M.M. Sherard, Q. Dang, J.S. Kaplan, J. Simpson, M.C. Leopold
- 165.** Exploring the bonding in ternary mercury dihalide clusters [Poster Board #165]. **N. Buell**, K. Donald
- 166.** Exploring the use of functionalized nanomaterials to combat the fentanyl opioid epidemic [Poster Board #166]. **M. Sherard**, J.S. Kaplan, K. Lalwani, Q. Dang, M.C. Leopold
- 167.** What clusters forget: Signs of bonding transitions in Group 12 metal dihalides (contrasted with van der Waals chains) [Poster Board #167]. **I. Mohren**, Z. Shafi, K. Donald
- 168.** Light sensitive ruthenium-based compounds as prodrugs for lung cancer [Poster Board #168]. **A. Wilson**, K. Enkbold, Y. Chung, S.L. Chiaino, M.R. Norris, J.A. Pollock
- 169.** Isomers of 2-pyridyl-naphthyridine ligands and their metal complexes [Poster Board #169]. **L. Simkins**, B. Solomon, M. Ortiz, R.N. Dominey, E.W. Goldman
- 170.** Alkali metal incorporation into Ir/Ru oxides for oxygen evolution from water splitting [Poster Board #170]. **Z.S. Moore**, M. Falsaperna, S. Freakley, A.G. Glenn, T.A. Nile
- 171.** Functional metal-organic frameworks-based sensing for the sensitive determination of heavy metals in polluted water [Poster Board #171]. **M.H. Kabir**, E. Ford, M. Shohag
- 172.** Preparation of PLGA for drug delivery [Poster Board #172]. **J. Bailey**, T. Vasicek
- 173.** Trimethylsilyl trifluoromethanesulfonate-promoted one-pot synthesis of 4-isoxazolines from chalcones and N-benzylhydroxylamine [Poster Board #173]. **G. Hughes**, C.W. Downey
- 174.** One-pot enol silane formation-alkylation reactions of ketones and (diaryl)methyl acetates [Poster Board #174]. **K. Marchione**, K. Smith, C.W. Downey
- 175.** Synthesis of beta-hydroxyamino alcohols from ketones [Poster Board #175]. **M. Strigel**, O. Lambertson, R. Goodner, C.W. Downey
- 176.** Propargyl amides from trimethylsilyl trifluoromethanesulfonate-promoted additions of secondary amides to propargyl propionates [Poster Board #176]. **R. Graff**, T. Chong, A. Helbling, C.W. Downey
- 177.** Exploration of benzothiazoles as cleavable Linkers [Poster Board #177]. **J. Blobe**, A. Dalton
- 178.** Synthesis of antibiotic-adjuvant conjugates [Poster Board #178]. **I.M. Starr**, A.L. Wolfe

- 179.** Synthesis and evaluation of 2-(methylthio)quinoline analogs to assess their viability as novel antibiotics against *Pseudomonas aeruginosa* [Poster Board #179]. **K. Ward**, R. Steed, A.L. Wolfe
- 180.** Synthesis and antibacterial evaluation of quinoline molecules capable of inhibiting ATP synthase in *Pseudomonas aeruginosa* [Poster Board #180]. **C.A. Blair**, **A.M. Chatterjee**, **A. Karthikeyan**, **A.S. Roper**, R. Steed, A.L. Wolfe
- 181.** Optimization of the synthesis of polyfunctionalized pyrroles using continuous flow techniques [Poster Board #181]. **K. Dwomoh**, **E. Ramirez**, J.T. Gupton, E.W. Goldman, R.N. Dominey
- 182.** Synthesis, polymerization, and investigation of hydrogen bonding of 4-vinylimidazole [Poster Board #182]. K. Caminiti, **T. Cosby**
- 183.** Comparison of adsorbed vs. covalently-bound immobilized cellulase to magnetic nanoparticles [Poster Board #183]. **C.D. Snavely**, T. Vasicek
- 184.** Proposing a new method for determining aromaticity through comparison of inclusive vs. non-inclusive steric number calculation in conjunction with an alternative approach to reveal conjugated pi systems in alkyne-containing compounds [Poster Board #184]. **D. Amiri**, V. St. Hilaire
- 185.** In silico exploration of the conformational space of biliverdin [Poster Board #185]. **T. Du**, E. Pieri
- 186.** Strain induced color change of cholesteric liquid crystal polymer ribbons [Poster Board #186]. **P. Latimer**, C. Tang
- 187.** Further examination of the recently proposed lone pair hybrid model to evaluate its validity in revealing conjugated pi systems in alkyne-containing compounds [Poster Board #187]. **D. Amiri**
- 188.** Investigating cosolvency through molecular simulations of “smart” stimuli-responsive long chain polymers [Poster Board #188]. **C. Vasnetsov**, V. Vasnetsov
- 189.** Conformational preferences in MX_2^{\pm} and MX_3^{\pm} systems as probes for bonding models [Poster Board #189]. **S. Redzic**, K. Donald
- 190.** Investigation of the S321A variant of the thiamine-dependent enzyme SucA in abiological carbon-carbon bond-forming reactions [Poster Board #190]. **S. Bibi**, E. Reynolds
- 191.** Analysis of writer gene expression data for RNA modifications found in glioblastoma [Poster Board #191]. **C. Eddings**, J.H. Simpson, R.L. Flemings, B.A. Tannous, N. Chiu

- 192.** Structural and biochemical comparison of *Francisella tularensis novicida* two component system response regulator proteins QseB, KdpE, and BfpR [Poster Board #192]. **K. Gaddy**, E.M. Bensch, J. Cavanagh, M. Milton
- 193.** CRISPR screen reveals microenvironment-specific radiosensitizing factors in glioma models [Poster Board #193]. **K. Long**, S. Floyd, D. Luo, R. Chen, A. Katz
- 194.** Identifying the metal-binding histidine residues of human serum albumin using hydrogen-deuterium exchange and mass spectrometry [Poster Board #194]. **C.E. Agwuegbo**, K. Haas
- 195.** Conformational analysis of a force-induced retro Diels-Alder reaction using DFT [Poster Board #195]. **F. De Araujo Ferreira**, G. Gomez, A.G. Roessler
- 196.** Analysis of the ashes of the peels of bananas grown in South Georgia [Poster Board #196]. **B. Miburo**
- 197.** Synthesis and characterization of carbon nanodots-protein conjugates for the treatment of bone disease [Poster Board #197]. **A. Ali**, Q. Chau, J.D. Dattelbaum, I. Skromne
- 198.** Synthesis of a large macrocyclic amine for enzyme mimic studies [Poster Board #198]. **V. Pham**, A. Lajmi
- 199.** Isolation and identification of compounds with antibiotic activity against ESKAPE pathogen relatives [Poster Board #199]. **H. Lwin**, S.G. Clarke, J.D. Dattelbaum
- 200.** Characterization of a putative periplasmic branched chain amino acid binding protein TM1135 from *Thermotoga maritima* [Poster Board #200]. **E. Kim**, S. Marsicano, J.D. Dattelbaum
- 201.** Use of a thermal shift assay to identify small molecule modulators of *staphylococcus aureus* STK1 and STP1 [Poster Board #201]. **C. Sung**, H.B. Miller, M.S. Blackledge, J.A. Pollock

Durham Arts Council
PSI Theatre

Inorganic Chemistry Research and Development

Cosponsored by INOR
D. A. Canelas, K. C. Glasgow, J. M. Harrington, *Organizers*

9:00 Introductory Remarks.

9:05. Hydrocarbon transformations at well-defined surface sites utilizing early transition metal precursors. **K. Searles**

9:20. Novel lanthanum hydroxyl borate structure with potentially deep-ultraviolet birefringent properties at extreme conditions. **O. Ibragimova**, L. Vaquero, Z. Hussein, S. Chariton, V. Prakapenka, I. Chuvashova

9:35. Development of highly active lithium metal for the synthesis of organolithium reagents. M. Crockett, **L.S. Aguirre**, L.B. Jimenez, H. Hsu, A.A. Thomas

9:50. Magnetic ordering in 3d metal intercalated VTe₂. **M. Adams**, C. Huang, M. Shatruk

10:05 Break.

10:15. Controlling product selectivity during dioxygen reduction with MN complexes using pendant proton donor relays and added base. **E.N. Cook**, I.M. Courter, D.A. Dickie, C.W. Machan

10:30. Divergent activation modes of silylpalladium cations: Mechanistic study of non-traditional metal-silyl reductions of ketones. **E. Roos**, M.R. Gagne

10:45. Ligand-functionalized InP-based quantum dots as photosensitizers in antimicrobial photodynamic inactivation. **L. Chen**, R.A. Ghiladi, C.B. Gorman, F. Scholle

11:00. Incorporation of proton transfer chain in metal-organic frameworks for improved water oxidation. **B. Thomas**, A.J. Morris

11:15 Break.

11:25. Light-initiated structural changes in ruthenium complexes bearing IR active groups that associate halide ions. **J. Dickenson**, G.J. Meyer

11:40. Comparative study of the crystal structures and synthetic techniques for the preparation of ternary hafnium/zirconium fluorides. **N. Keerthisinghe**, H. zur Loye

11:55. Exploration, prediction, and experimental verification of structure and properties in defect-resistant I₂-Eu-IV-X₄ (I = Li, Cu, Ag; IV = Si, Ge, Sn; X = S, Se) chalcogenide semiconductors. **T.M. McWhorter**, T. Wang, D.B. Mitzi, V. Blum

Durham Arts Council
Duke Rehearsal Hall

K12 Educators Day

Cosponsored by CELL, CHAS and CHED
M. B. Koza, L. S. Sremaniak, *Organizers*

9:00 Managing Chemicals Safety Workshop.

11:30. Probing at the interpretations, implementations, and assessments of information literacy in chemistry/science education classrooms by K-12 teachers in Central Florida. **C. Randles, M. Lam**

12:00 Awards Lunch.

1:00 New NC High School Standards.

1:30. Doing safe and fun chemistry. **A.A. Hazari**

Durham Convention Center
Junior Ballroom C

Organic Chemistry Research and Development

D. A. Canelas, K. C. Glasgow, *Organizers*
J. Poutsma, *Presiding*

9:00 Opening Remarks.

9:05. Identifying the factors which control oxazalone versus diketopiperazine fragmentation in APA peptides. **J. Poutsma**, S.E. Farmer, S.M. Glass, L.J. Quirarte Hutton, V.H. Wysocki, J.C. Poutsma

9:20. Total chemical synthesis and bioactivity of novel antibacterial peptides from *capsicum chinense* X *frutescens*. **Z. Brown**, S. Mitchell, K.D. Culver, L.N. Shaw, L.M. Hicks, A.J. Wommack

9:35. Exploring the reactivity of azapeptides through late-stage functionalization. **M. Bowles**, C. Proulx

9:50. Evidence for single electron transfer in monoamine oxidase: A biomimetic study. **N. Price**, J. Tanko

10:05 Break.

10:15. New method for cyclic peptide synthesis using hydrazone linkages with high side chain diversity. **E.J. Warner**, Q. Guthrie, B. Humphrey, C. Proulx

10:30. Chemical investigation of coral-associated probiotic bacteria. **E. Smith**, A. Peñuela Mendoza, M. Walter, M.L. Van Hoek, P. Videau, R.T. Williamson, B. Ushijima, W.K. Strangman

10:45. Manufacture on scale of custom-made non-natural amino acids. **T.T. Romoff**, B. Marchyshyn, A. Smith, T. Gordon, S. White, A. McNeill, G. Butler

11:00. Next generation of vancomycin antibiotics. **A. Valdes**, J.G. Pierce

Durham Convention Center
Junior Ballroom D2

Polymer Chemistry and Materials Science Research and Development

Cosponsored by PMSE and POLY
D. A. Canelas, *Organizer*
T. Cosby, J. Sternberg, *Presiding*

9:00 Introductory Remarks.

9:05. Ion dynamics and charge transport in imidazolium ionic liquids. **T. Cosby**, C.D. Stachurski, D.P. Durkin, R.A. Mantz, P.C. Trulove

9:20. Interfacial passivation of perovskite solar cells by imidazolium ionic liquids. **R. Panta**, C.A. Grapperhaus, T. Druffel

9:35. Oligo(ethylene glycol) side chain architecture enables alcohol-processable conjugated polymers for organic solar cells. **J. Neu**, W. You

9:50 Intermission.

10:00. Chemical recycling of post-consumer PET and synthesis of renewable semi-aromatic polyamides. **J. Sternberg**, S. Pilla, B. Guin, O. Sequerth

10:15. Rapid nano-viscometer, *nanovisQTM*, measures shear thinning at high shear. **D. French**, M. Bonner, Z. Parlak

10:30. Improving the wet lubricity of polyethylene using tribological methods. **B. Singhi**, J.R. Campanelli

10:45. Developing a functional finish based on cottonseed oil. **T.A. Kanipe**, L. Meza Carvajal, H. Chang, S. Park, R. Venditti

11:00 Intermission.

11:10. *In-situ* sequential solution polymerization of conductive polyaniline films for three-terminal memristors as neuromorphic/integrated circuits. **T. Wanless**, B. Grant, I. Bandera, S.H. Foulger

11:25. Synthesis of *N*-heteroacenes towards applications in organic electronics. **I. Cockman**, C.B. Gorman

11:40. Photoelectrochemical valorization of biomass derivatives with hematite photoanodes modified by CoPi catalyst. **S. Grandi**, I. Carrai, R. Mazzaro, E. Bassan, G. Morselli, A. Piccioni, S. Caramori, P. Ceroni, L. Pasquini

Durham Convention Center
Junior Ballroom A2

Southeastern Magnetic Resonance Conference (SEMRC)

Cosponsored by ANYL and PHYS
A. I. Smirnov, M. A. Ter Horst, *Organizers*

9:00 Introductory Remarks.

9:05. Opportunities of multi-electron DNP with sub-nanometer e-e distances. **S. Han**

9:25 Q&A with Dr. Han.

9:35. Structural model for a 32-mer oligomer of the Alzheimer's amyloid- β peptide. Y. Gao, A. Robang, R. Prasad, P. Randolph, J. Watzlawik, C. Guo, S. Stagg, H. Zhou, T.L. Rosenberry, **A.K. Paravastu**

9:50. Exploration of ¹⁹F-QNMR in tapping the functions of GPCR intermediate conformational states. **L. Ye**, x. wang, M. Bi, C. Neale, S. Kim, W.A. Goddard, Y. Cheng, Y. Miao

10:05 Break.

10:15. Controlled confinement effects on solvent-coupled protein dynamics in monomeric, oligomeric, and fibrillar α -synuclein. **K. Whitcomb**, K. Warncke

10:30. Multifaceted membrane interactions of human Atg3 promote LC3-phosphatidylethanolamine conjugation during autophagy. **f. tian**, Y. Ye, V. Bui, H. Wang

10:45. Membrane composition drives sidechain ionization and assembly of transmembrane protein domains: Potential implications for TCR assembly. **T. Smirnova**, M.A. Voinov, S. Milikisiyants, G. Cook, A.I. Smirnov

11:00 Break.

11:10. Hyperpolarization chemistry for precision measurements and molecular imaging. **T. Theis**

11:25. Using DFT simulations for co-ligand design to fine-tune the exchange rate of polarization targets in SABRE. **F.V. Tran**

11:40. Enabling the broad class of alpha-keto acids as SABRE hyperpolarization targets and exploring their polarization dynamics. **S. McBride**, K. Macculloch, P. TomHon, A. Browning, E. Chekmenev, T. Theis

11:55. PhIP ¹³C radiofrequency amplification by stimulated emission of radiation. **C. Nelson**, A. Schmidt, I. Adelabu, S. Nantogma, V. Kiselev, A. Adburraheem, H. de Maissin, S. Lehmkuhl, S. Appelt, T. Theis, E. Chekmenev

Durham Convention Center
Meeting Room 4

Analytical Chemistry Back in the Classroom/Lab: Pedagogy We Learned from Teaching Online

Cosponsored by ANYL and CHED
Z. S. Davis, G. E. Potts, *Organizers*

9:30 Opening Remarks.

9:35. Internal standard or standard addition? Addressing the effects of Covid on the student matrix and course-to-course variability at Christopher Newport University. **R.A. Quinlan**, A. Higgs

9:50. Bridged course-embedded undergraduate research experiences for analytical and instrumental chemistry: Assessment of impacts on technical skills. **K. Zimmermann**, R. Simmons, X. Li, W. Huang, Y. Guo, R.K. Kalman, S. Mwongela, M. Anzovino, C. Brown, R. Fiorrillo

10:05. Enhancing analytical chemistry education through online pedagogy. **F. Yan**

10:20 Intermission.

10:30. Engaging quantitative analysis students in an active learning environment. **G.E. Potts**

10:45. Activities to promote active learning in the quantitative analysis course. **L. De La Garza**

11:00. Teaching post-pandemic analytical chemistry lecture and laboratory: Improving student abilities of problem-solving and data treatment. **W. Zhou**

11:15 Panel Discussion.

Durham Convention Center
Junior Ballroom A1

Chemistry Education Research: Undergraduate Student Research Symposium

Cosponsored by CHED
D. A. Canelas, *Organizer*
C. T. Cox, *Presiding*

9:30 Introductory Remarks.

9:35. Analysis by GCMS of the extracts of the straws and pine cones of longleaf pine trees of South Georgia. **B. Miburo**

9:50. Exploring the mechanism of a RuO₄-catalyzed system for oxidation of benzyl silyl ethers. **A.G. Riccardi**, M.L. Turley, A.M. Weinhofer, C. Rigsby, M. McKenna, A.L. Moser, B.C. Goess, S.K. Goforth

10:05. Optimization of fluorescence correlation spectroscopy (FCS): Characterization of novel fluorophores. **J.M. Dixon**, K. Fogarty, P. Lundin, A. Pierre

10:20 Intermission.

10:30. Synthesizing and characterizing a library of rhodamine B amide dimers with varying covalent linkers. **A. Pierre**, R. Spera, B. Stratton, K. Fogarty, P. Lundin

10:45. Determining the binding of Pyronin Y with cucurbit[8]uril using constant constrain analysis. **M. Keeler**, P. Ramirez Fernandez, J.E. Hansen, F.A. Khan

11:00. Structural dynamics within the *Escherichia coli* ATP synthase complex. **B. Chavez-Arellano**, E. Dowdall, R. Steed

11:15 Intermission.

11:25. Transcriptomic analyses of multiple antibiotic adjuvants against MRSA. **R. Stempel**, H. Balogh, B. Viering, M.S. Blackledge, H.B. Miller

11:40. Inhibiting ATP synthase with quinoline antibiotics causes cell death in multidrug resistant *Pseudomonas aeruginosa*. **A. Williams**, R. Steed, A.L. Wolfe

11:55. The role of subunit *a* lysine 203 on proton translocation in *E. coli* ATP synthase. **A. Gaspar-Rivera**, R. Steed

Durham Arts Council
Adaron Hall

Ultrafast and Nonlinear Spectroscopy

Cosponsored by ANYL
E. Ghadiri, L. Wang, *Organizers*
R. F. Ribeiro, *Presiding*

10:00 Introductory Remarks.

10:05. Solvent-driven helix-coil transitions in chiral conjugated polymers. **L.A. Peteanu**, Y. Shang, E.T. Smith, D. Sharma, K.J. Noonan, T. Kowalewski, M. Cotlet

10:25. Radical ion excited states: Extraordinary photophysics from ordinary chromophores. **B. Kudisch**

10:45. A brief history of stimulated Raman scattering microscopy and an update on recent work. **R.C. Prince**, E. Potma

11:05 Intermission.

11:15. Albumin-bound “switch-on” near-infrared emission beyond dark pigment absorption for forensic latent blood detection. M. Saucier, **N. Kruse**, T. Lewis, W.E. Meador, N. Hammer, J.H. Delcamp

11:35. Ultrafast propagation of excitons in polaritonic quantum wires. **G. Aroeira**, K. Kairys, R. Florentino Ribeiro

11:55. Investigating photodynamics of the double well triplet state in 2-Thiothymine through wavelength dependent time-resolved photoelectron spectroscopy. **Y. Qu**, S. Ullrich

Durham Convention Center
Grand Ballroom I

Project SEED Poster Session

Cosponsored by CHED
A. Mallia, *Organizer*

10:40 - 12:40

147. SEED Scholarship Program - Who can apply and how? [Poster Board #147]. **J.F. Rubinson**

148. Efforts toward crystallization induced processes of β -dicarbonyls [Poster Board #148]. **M. Saeed**

149. Electronic structure and reactivity of Cp*iriii complexes: Leveraging hemilability to unlock new reactivity [Poster Board #149]. **A. Mahadeshwar**

150. Chemical-genetic interactions that affect cell and chloroplast division in *Chlamydomonas reinhardtii* [Poster Board #150]. **A.L. Perry**

151. Green Synthesis of voxelotor [Poster Board #151]. **A.G. Martinez-Lopez**

152. Qualitative determination of heavy metals through the use of Tetra hydroxyphenyl porphyrin-doped silica sol-gels [Poster Board #152]. **M. Collins**, C.H. Lisse

153. Synthesis and reactivity of new N-heterocyclic thiones and selones [Poster Board #153]. **C. Davis, E.P. Huemmer**, M.J. Zelada-Bazán, D. Rabinovich

154. Synthesis, purification, and photophysical studies of 4-(1-naphthylazo)phenol [Poster Board #154]. **K. Lin**, A. Mallia

155. Preparation of sulfur salts for the synthesis of cyclobutanone derivatives via ring expansion of cyclopropanone adducts [Poster Board #155]. **A. Oudeh**, J.E. Muir, V. Lindsay

156. Synthesis and gelation studies of ammonium Alkanoates as low molecular mass gelators [Poster Board #156]. **H.G. Kunwar**, J. Suazo, A. Mallia

157. Synthesis of achiral squaramide organocatalysts for the screening of new reactions [Poster Board #157]. **E. Choi**, Q. On, H.S. Hinton, T.M. Parsons, J.E. Brown, J.A. Pigza

158. The antibacterial and antioxidant evaluation of calycosin [Poster Board #158]. **H. Boakye**

159. Engineering polyketide synthase (PKS) pathways for derivatized natural products [Poster Board #159]. **J. Matondo**

160. Exploring the reactivity of N-aryl peptides in organic solvents [Poster Board #160]. **S. Gage**, C. Proulx, K. McKinney, E.J. Warner

161. Expanding the substrate scope of the thiamine-dependent enzyme alpha-ketoglutarate dehydrogenase through strategic mutations: A structure-based approach [Poster Board #161]. **J. Perez-Hernandez**, E. Reynolds

162. Synthesis, structure-property relationship, and gelation studies of ortho, meta, and para isomers of (Hydroxyphenyl)alkanamides [Poster Board #162]. **W. Ibrahim**, B. Fisher, A. Mallia

163. Optimization of microwave-assisted extraction of cyclotides and purification using HPLC [Poster Board #163]. **J. Lee**, J. Suazo, B. Fisher, N.Y. Forlemu, S. Mwongela, S. Tangirala, A. Mallia

164. Effect of alkyl chain length on the 4-alkyloxycoumarin and 7-Alkoxy coumarin derivatives as low molecular mass gelators [Poster Board #164]. **J. Leonora**, N. Le, A. Mallia

165. Reimagining qualitative organic chemistry through course-based undergraduate research experiences (CURE) [Poster Board #165]. **S.M. Cooper**

Durham Convention Center
Grand Ballroom I

Undergraduate Poster Session

Cosponsored by CHED
J. A. Feducia, K. C. Glasgow, *Organizers*

10:40 - 12:40

101. Incorporation of an unnatural amino acid into Memo1 [Poster Board #101]. **S. Mecorapaj**, J.A. Pollock

102. Extending the wavelength of photosensitive click substrates [Poster Board #102]. **F.A. Stolpen**, P.B. Jones, L. Wood, Y. Zhu

103. Synthesis of pyrazole derivatives and pyrazolato-based polynuclear iron complexes [Poster Board #103]. **N. Pino**, **D. Rodriguez**, **S. Serrano**, A.J. Rodriguez

104. Solar phototransformation of melatonin in simulated aquatic environments [Poster Board #104]. **A. Rovinski**, W. Cory

105. Investigating the photocatalytic reduction of alkynes using an organic photocatalyst [Poster Board #105]. **R.A. Wernsman**, J.M. Hanna

106. Determination of poly(vbTMAC) extinction coefficient at various lengths and solutions [Poster Board #106]. **D. Desai**, J.C. Poler

107. Structural and functional characterization of EToV nuclease nsp12 [Poster Board #107]. **J. Fleming**, P. O'Reilly

- 108.** Utilizing a palladium-catalyzed dehydration of a primary amide toward the synthesis of vildagliptin [Poster Board #108]. **G. Develle**, J. Stanley, K. Alam, M.P. Croatt
- 109.** Characterization of Memo1 protein-protein interactions [Poster Board #109]. **H. Salus**, C. Bayas, J.A. Pollock
- 110.** Diversifying oxetanes: Expanding the scope of the Paternò-Büchi reaction [Poster Board #110]. **F. Green**, S. Coote, A.G. Glenn, T.A. Nile
- 111.** Evaluating prototype Uniqsis photoreactors with a benzylic bromination [Poster Board #111]. **G. Rich**, J. Tibbetts, A. Cresswell, T.A. Nile, A.G. Glenn
- 112.** Using molecular dynamic simulations to examine molecular behaviors of biomass derivatives as an alternative solution to crude oil feedstock [Poster Board #112]. **K. Yard**, A. O'Malley, K. Morton, A.G. Glenn, T.A. Nile
- 113.** cerium(IV) mediated hydrolysis of cyclic di-GMP: A potential strategy to enhance antibiotic performance against bacteria [Poster Board #113]. **S. Landers**, D.E. Williams
- 114.** Cloning of an algal aquaporin gene into *E. coli* [Poster Board #114]. **A. Madrigal Olivarez**, D.L. Gosnell
- 115.** Optimization of DNA extraction for genome sequencing of the invasive mussel *Mytella charruana* [Poster Board #115]. **J.C. Adams**, C. Calestani
- 116.** Identifying mutants of the de novo protein S824 as capping ligands for the biosynthesis of CDs quantum dots [Poster Board #116]. **V.L. Payne**, L. Spangler
- 117.** Detection of the reactive species in cellular culture [Poster Board #117]. **C.W. Francis**, Y.Y. Woldman
- 118.** Metals quantification in American wines [Poster Board #118]. **L. Atilano**, **J. Autry**, P. Jacoby, J.D. Leyba
- 119.** Backyard chicken exposure to lead in Spartanburg, SC [Poster Board #119]. **L. Vane**, M. Gilliland, L. Cruze, G.E. Schwartz
- 120.** Analytical determination of iron and manganese concentrations in raw and filtered North Georgia well water via total reflection x-ray fluorescence [Poster Board #120]. **R. Rowland**, S. Clark, R.N. Dansby-Sparks, L.J. Wilson
- 121.** General use of solid-state indicators [Poster Board #121]. **S. Starnes**, S.K. Hutchison, J.W. Hall
- 122.** Modular approach to prescreening prodrugs of a potent platinum-acridine anticancer agent [Poster Board #122]. **D. Coffin**, L. Sapp, U. Bierbach

- 123.** Crystal growth of oxides and fluorides using molten salt flux's [Poster Board #123]. **V. Jones**, G. Morrison, H. zur Loye
- 124.** Optimizing the microwave reaction of europium-doped calcium fluoride nanoparticles [Poster Board #124]. **J. England**, M. Fratarcangeli, C.R. De Silva
- 125.** Increasing the scope of pharmaceutical compounds containing functionalized seven-membered carbon rings: Applications in synthetic organometallic chemistry [Poster Board #125]. **R. Stegner**, M.N. Ericson, W. Harman
- 126.** Comparison of silyl sulfides as precursors for SnS nanocrystal growth [Poster Board #126]. **M. Henley**, J. Desormo, J. Bernard, M.R. McPhail
- 127.** Self-reporting CPNs for superoxide generation and detection [Poster Board #127]. E.J. Harbron, **A. Clayborn**
- 128.** The synthesis and characterization of end-group modified poloxamers [Poster Board #128]. **N. Ferguson**, R.J. Harris
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- 130.** Diaryl oxazoles: Oxidatively cleavable linkers for small molecule drug discovery platforms [Poster Board #130]. **E. Taggart**, **E. Wolff**, P. Yanar, C.R. Shugrue
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- 132.** Synthesis and characterization of opioid agonist and antagonist derivatives containing a Sonogashira linkage [Poster Board #132]. **L.E. Griffin**, M. Goertzen, T.L. McGomery, K.R. Boykin, K.R. Wilson
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- 134.** Utilizing the Brook rearrangement to form γ -keto oximes and their silyl enol ethers from acylisoxazolines [Poster Board #134]. **M.E. Paul**, **J.S. Sypolt**, A.M. Hartel
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- 137.** Extraction of carotenoids using ionic and non-ionic deep eutectic green solvents [Poster Board #137]. **D.B. Vasquez**, L. Rubio, I. Najar, A.L. Focsan, G. Sreenilayam

- 138.** Utilizing the Glaser-Hay coupling to generate a library of biologically active polyynes [Poster Board #138]. **B. Flood, S. Kregenow,** D.D. Young
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- 140.** Rapid machine learning classification of single-molecule organic fluorophores for blinking-based multiplexing [Poster Board #140]. **A.G. Seabury,** G.R. Hoy, G. DeSalvo, A. Khodabocus, K.L. Wustholz
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- 142.** Labeling density and power dependence of blinking-based multiplexing: Optimizing a new tool for multicolor single-molecule imaging [Poster Board #142]. **E. Smith,** S. Haile, G. DeSalvo, K.L. Wustholz
- 143.** Diffusion of limonene into paraffin wax with transmission Fourier-transform infrared spectroscopy [Poster Board #143]. **T. Gregory, M. Higgins,** C. Mitchell, S.W. Huffman
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